HIGH-END COMPUTING CAPABILITY PORTFOLIO

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NASA Advanced Supercomputing Division

January 10, 2022

National Aeronautics and Space Administration

ESS Launches Hyperconverged Infrastructure, Allowing Virtual Systems as a Service

- The Engineering Systems and Services (ESS) team completed the first phase of a multiphase initiative to introduce a core hyperconverged Infrastructure (HCI) solution to the HECC environment for Virtual Systems as a Service (VSaaS), providing numerous benefits:
  - Centralizes and simplifies management of virtual machines.
  - Greatly increases flexibility and scalability by managing a single pool of homogeneous compute resources.
  - Lowers costs and simplifies procurement of systems.
  - Improves security operations in monitoring and patching.
  - Establishes best practices and tools for configuration management and automation.
  - Significantly speeds up initial deployment of preapproved virtual system platforms.
- Phase 1 allows existing virtual machines to be hosted on the VSaaS. Subsequent phases will expand the HCI system and capabilities.
- This approach is a modern departure from existing legacy infrastructure with disparate physical servers, virtual machines, and services; noncentralized siloed storage attached to select servers; and heavily manual and lengthy processes to build systems.

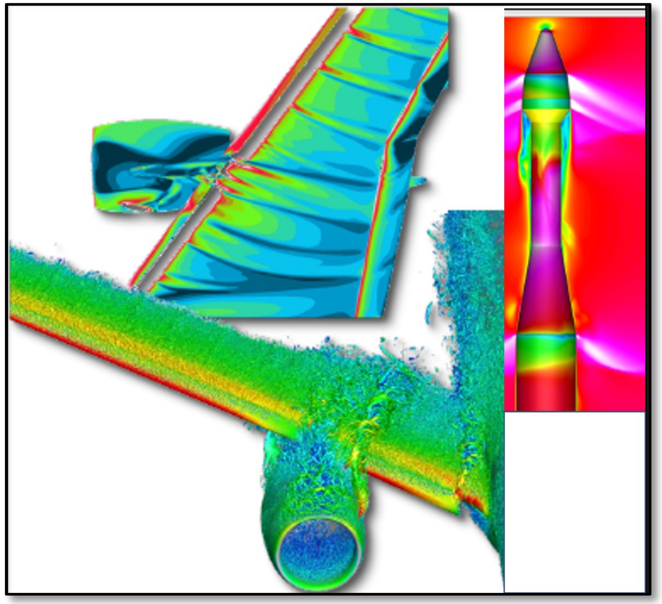
IMPACT: The VSaaS using HCI technology will form the foundation for HECC to provide modern enterprise-grade infrastructure servers, allowing systems to be deployed and managed in a fraction of the time that existing systems require.

3D rendering of a single VxRail E-Series node, the solution HECC selected to provide HCI capabilities to the NASA Advanced Supercomputing facility. This solution comprises four VxRail E-Series nodes in an N+1 high-availability configuration. *Dell EMC*

Exploring GPU Technology for Production CFD Workflows

- HECC recently requested a feasibility assessment from a select test group for migrating typical FUN3D user workflows to GPU hardware.
  - The GPU capability has had strong impact at other HPC facilities and across external organizations over the past three years.
  - HECC is providing a three-month reservations of 30 GPU nodes, each node equipped with four NVIDIA V100 GPUs, for the assessment.
- The FUN3D development team is shepherding several existing projects through a transition to GPU technology, including:
  - Aeroacoustic analysis supporting the upcoming Artemis I mission (HEOMD).
  - High-lift aerodynamics (ARMD).
  - Transonic buffet environment for launch vehicles (NESC).
- Applications are attaining 3 to 4.5 times speedup for one V100 GPU versus an Intel Xeon Skylake node, depending on workflow specifics.
- Additional projects will be migrated, pending hardware availability.
- The development team continues to pursue implementation and optimization for current and next-generation hardware technologies.

IMPACT: GPU technologies are making inroads across the HPC landscape and offer the potential to deliver improved application performance at reduced cost.

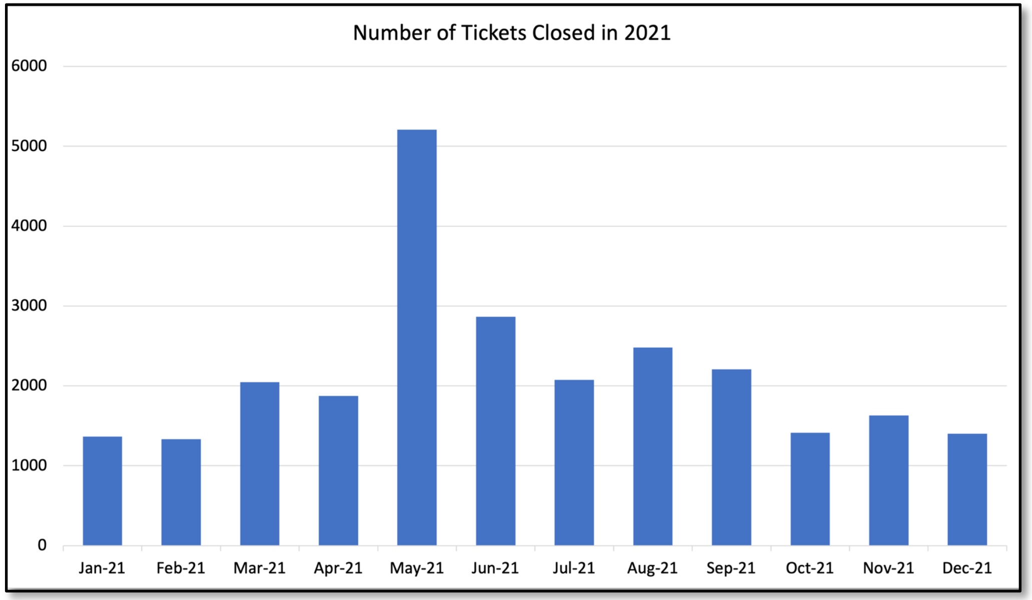


Images from some efforts leveraging the dedicated NAS GPU resources. High-lift flows: Reynolds-averaged Navier-Stokes modeling (left) and Wall-modeled large eddy simulation (right). *Li Wang, Nashat Ahmad, and Craig Streett, NASA/Langley*

Control Room Staff Continue Excellent Service to Users

- In 2021, HECC Control Room staff provided support to more than 1,500 users from all of NASA's mission directorates. Control Room staff processed, tracked, and resolved over 26,000 tickets for the 12 months from January 1 through December 31.
- Tickets covered a wide range of support activities—from automated notifications of system issues to resolving a variety of issues for users calling for help:
  - Answered inquiries about accounts, failed jobs, and status of systems.
  - Extended runtimes of already-queued or running jobs.
  - Created complex reservations for mission-critical projects.
  - Modified allocations and account expiration dates.
  - Explained file transfer tools and processes.
  - Debugged job failures and identified execution bottlenecks.
- In addition, the Control Room continued onsite support for internal support staff who are still working remotely from home due to COVID-19 access restrictions.
- The Control Room staff, with the Facilities team, was awarded an Ames Safety Award for their effective safety walkthroughs in in buildings N258 and N233A and the modular data center sites since the start of the Ames COVID-19 access restrictions.

IMPACT: The 24x7 support services provided by HECC Control Room Analysts resolve system problems and users' technical issues and enable users to focus on their important mission projects.

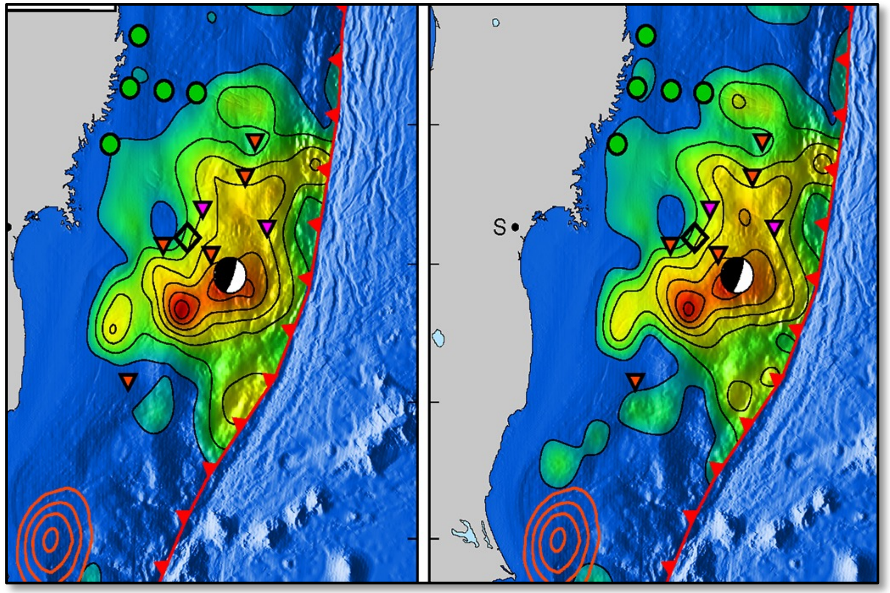


HECC Control Room staff resolved, on average, more than 2,150 Remedy tickets per month in 2021—just over 26,000 tickets total.

Applications Team Adds GPU Support to Earthquake Modeling Code

- The Applications Performance and Productivity (APP) team recently worked with US Geological Survey (USGS) researchers to port several compute-intensive kernels of their Cascading Adaptive Transitional Metropolis in Parallel (CATMIP) code to execute on GPU nodes at the NAS facility.
  - The original CATMIP code was developed at USGS for the estimation of finite fault earthquake source models. It employs MPI parallelization for multi-core CPUs and uses the Basic Linear Algebra Subroutine (BLAS) library. The performance is memory-bound.
- The goals of this effort were to assess the potential to use GPUs by adding GPU offload functionality to the application using CUDA and to transfer knowledge of those techniques to the USGS developers.
- The teams compared the runs on a single V100 GPU with those on a Skylake node using 35 CPU cores. Results showed:
  - Speedups of 20X to more than 100X on the single GPU for the compute-intensive kernels, depending on the test case.
  - Overall GPU performance is highly impacted by GPU-to-CPU memory traffic. This will likely improve as more parts of the code are ported to the GPU.
- APP will continue collaborating with USGS to fully port the application to the GPU with the goal of fitting submeter-resolution datasets available for recent California earthquakes.

IMPACT: Porting codes to run on GPUs has the potential to substantially decrease the cost of running applications on HECC resources. Considering the number of applications on HECC systems, teaching users how to port their codes is essential.



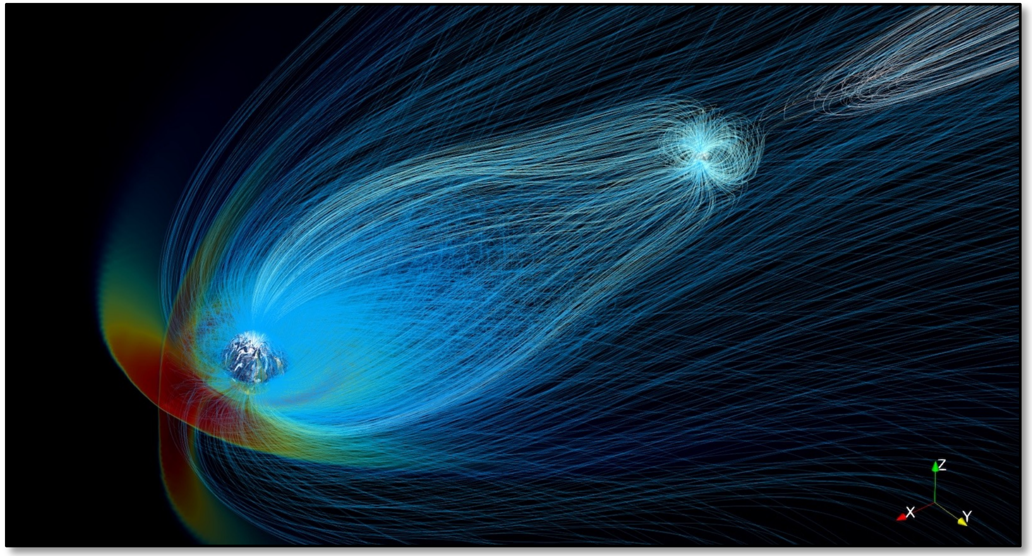
Because earthquake slip is uncertain, instead of making a single slip model, ~60 billion earthquake ruptures were modeled that are consistent with the observed surface deformation. The average slip over these billions of simulations is shown for time-independent (left) and time-dependent (right) models. *Minson et al., GJI, 2014*

Modeling Young Sun's Role in Lunar Ice and Hematite Deposits*

- After decades of study, it has been confirmed that water is present on the Moon's surface, mostly concentrated at the polar regions. Similarly, the mineral hematite has been found exclusively at the polar caps, leading researchers to wonder why.
- A team at Princeton University ran simulations of the interaction between a solar superstorm and the Earth-Moon magnetic field to better understand the formation of lunar polar ice and hematite and to determine the associated proton and ionospheric heavy oxygen ion fluxes falling on the lunar surface.
- Given that the young Sun was very magnetically active, the research focused on producing first-of-their-kind 3D multifluid magnetohydrodynamic simulations of the entire magnetized Earth-Moon during an extreme "Carrington-type" space weather event—also known as a solar superstorm.
- The simulations show how the magnetic field of the ancient Earth and Moon, in combination with a volatile young Sun, could have caused the lunar surface to be bombarded by solar storm protons and the Earth's ionospheric oxygen protons, especially at the poles, leading to large deposits of water and oxidization-derived hematite.

** HECC provided supercomputing resources and services in support of this work.*

IMPACT: The ability to simulate solar proton and Earth wind fluxes on the lunar surface—and comparing results with remote sensing data—could revolutionize our understanding of the origin of volatile compounds (such as water) on planetary bodies within the inner solar system.



3D representation of the entire magnetized Earth-Moon system during an extreme "Carrington-type" space weather event, where the Moon is behind the Earth. Color contours depict the total fluid pressure in nanoscale, while the cyan lines represent magnetic fields through which oxygen ions can be transported from Earth to the lunar poles. *Chuanfei Dong, Liang Wang, Princeton University*

CFD Analysis of Integrated Propulsion Systems for the SUSAN Aircraft*

- Researchers in the NAS Division performed CFD simulations to support the development of the SUbsonic Single Aft eNgine (SUSAN) concept, a hybrid electric transport aircraft designed to help address environmental issues faced by the aviation industry.
- The team used the Launch Ascent Vehicle Aerodynamics (LAVA) curvilinear solver for the Reynolds-Averaged Navier-Stokes (RANS) equation. LAVA's actuator zone method was used to model the effect of each propulsor on the airframe aerodynamics.
  - The focus was to gain insight into the impact of the airframe aerodynamics on the performance of each propulsion system, quantifying thrust, efficiency, and inlet distortion.
  - Analyses were performed for an aft fuselage turbofan and wing-mounted distributed electric propulsors, each developed for boundary-layer ingestion.
- Understanding the impact that the integration has on the external aerodynamics of the airframe gives engineers a better idea of how to efficiently integrate the propulsors with the aerodynamic surfaces to enhance lift, reduce drag, and improve propulsive efficiency.

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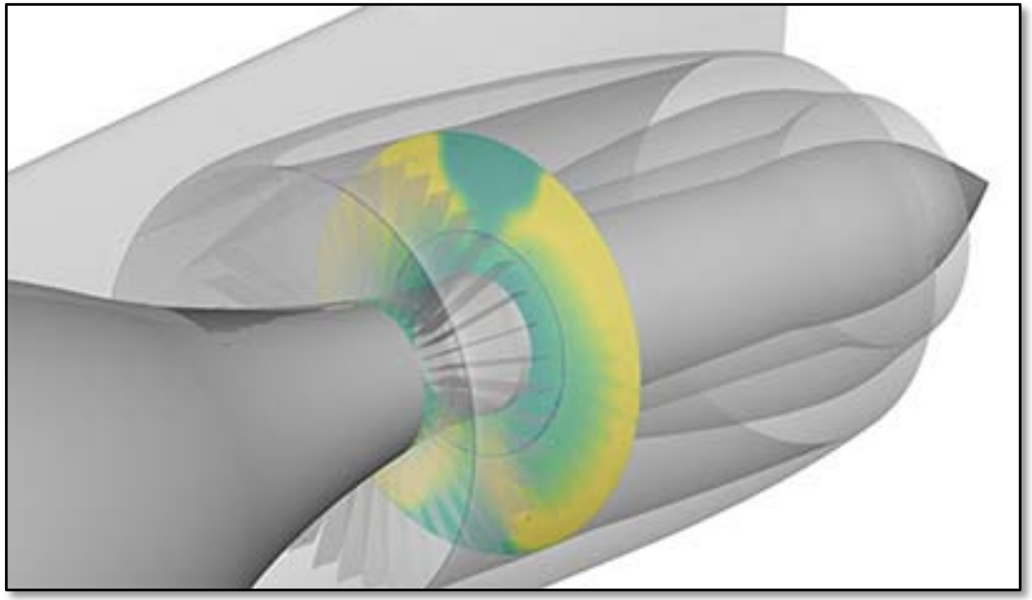
IMPACT: The SUSAN simulation results, made possible by HECC resources, help guide the design efforts for investigating novel integrated propulsion systems that can provide significant improvements to aircraft efficiency.



Total pressure contours downstream of the aft fuselage turbofan inform engineers how boundary-layer ingestion and inlet distortion impact propulsive efficiency, while providing insight into the benefits of inlet guide vanes and aft fuselage shape optimization.
Jared Duensing, Leonardo Machado, Timothy Chau, NASA/Ames

Papers

- "**TOI-1842b: A Transiting Warm Saturn Undergoing Re-Inflation Around an Evolving Subgiant**," R. Wittenmyer, et al., arXiv:2112.00198 [astro-ph.EP], December 1, 2021. *
  https://arxiv.org/abs/2112.00198
- "**GJ 367b: A Dense, Ultrashort-period Sub-Earth Planet Transiting a Nearby Red Dwarf Star**," K. Lam, et al., Science, vol. 374, issue 6572, December 2, 2021. *
  https://www.science.org/doi/abs/10.1126/science.aay3253
- "**Continuum to Rarefied Diffusive Tortuosity Factors in Porous Media from X-ray Microtomography**," J. Ferguson, et al., Computational Materials Science, vol. 203, published online December 3, 2021. *
  https://www.sciencedirect.com/science/article/abs/pii/S092702562100714X
- "**Modeling Ion Beams, Kinetic Instabilities, and Wave Observed by the Parker Solar Probe near Perihelia**," L. Ofman, et al., arXiv:2112.02357 [astro-ph.SR], December 4, 2021. *
  https://arxiv.org/abs/2112.02357
- "**Thermal Forcing of the Nocturnal Near Surface Environment by Martian Water Ice Clouds**," B. Cooper, et al., Journal of Geophysical Research: Planets, vol. 126, issue 12, December 5, 2021. *
  https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2020JE006737

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

- ”**Transit Timings Variations in the Three-Planet System: TOI-270**,” L. Kaye, et al., Monthly Notices of the Royal Astronomical Society, accepted manuscript, published online December 6, 2021. *
https://academic.oup.com/mnras/advance-article-abstract/doi/10.1093/mnras/stab3483/6454033
- “**Photospheric Prompt Emission From Long Gamma-ray Burst Simulations. I. Optical Emission**,” T. Parsotan, D. Lazzati, The Astrophysical Journal, vol. 922, no. 2, December 6, 2021. *
https://iopscience.iop.org/article/10.3847/1538-4357/ac2428
- “**Characterization of Magneto-Convection in Sunspots: The Gough-Tayler stability criterion in MURaM Sunspot Simulations**,” M. Schmassmann, et al., Astronomy & Astrophysics, vol. 656, December 7, 2021. *
https://www.aanda.org/articles/aa/abs/2021/12/aa41607-21/aa41607-21.html
- “**The Carbon Cycle of Southeast Australia During 2019-2020: Drought, Fires, and Subsequent Recovery**,” B. Bryne, et al., AGU Advances, vol. 2, issue 4, December 9, 2021. *
https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2021AV000469
- “**Cosmology with the Roman Space Telescope—Synergies with CMB Lensing**,” L. Wenzl, et al., arXiv:2112.07681 [astro-ph.CO], December 14, 2021. *
https://arxiv.org/abs/2112.07681

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Papers (cont.)

- “**Could the Magnetic Star HD 135348 Possess a Rigidly Rotating Magnetosphere?**” R. Jayaraman, et al., arXiv:2112.07676 [astro-ph.SR], December 14, 2021. *
  https://arxiv.org/abs/2112.07676
- “**Computation of Conventional and Alternative Jet Fuel Sensitivity to Lean Blowout**,” V. Hasti, et al., Journal of the Energy Institute, vol. 101, published online December 15, 2021. *
  https://www.sciencedirect.com/science/article/abs/pii/S1743967121002129
- “**Stochastic Guidance of Buoyancy Controlled Vehicles under Ice Shelves using Ocean Currents**,” F. Rossi, et al., 2021 IEEE/RSJ International Conference on Intelligent Robots and Systems, Prague, Czech Republic, September 27-October 1, 2021, published online December 16, 2021. *
  https://ieeexplore.ieee.org/abstract/document/9635987
- “**Numerical Simulations and Analysis of the Turbulent Flow Field in a Practical Gas Turbine Engine Combustor**,” V. Hasti, et al., Proceedings of the Institution of Mechanical Engineers: Journal of Power and Energy, December 21, 2021. *
  https://journals.sagepub.com/doi/abs/10.1177/09576509211063255
- “**Exosphere Modeling of Proxima b: A Case Study of Photochemical Escape with a Venus-like Atmosphere**,” Y. Lee, C. Dong, V. Tenishev, The Astrophysical Journal, vol. 923, no. 2, December 21, 2021. *
  https://iopscience.iop.org/article/10.3847/1538-4357/ac26bb

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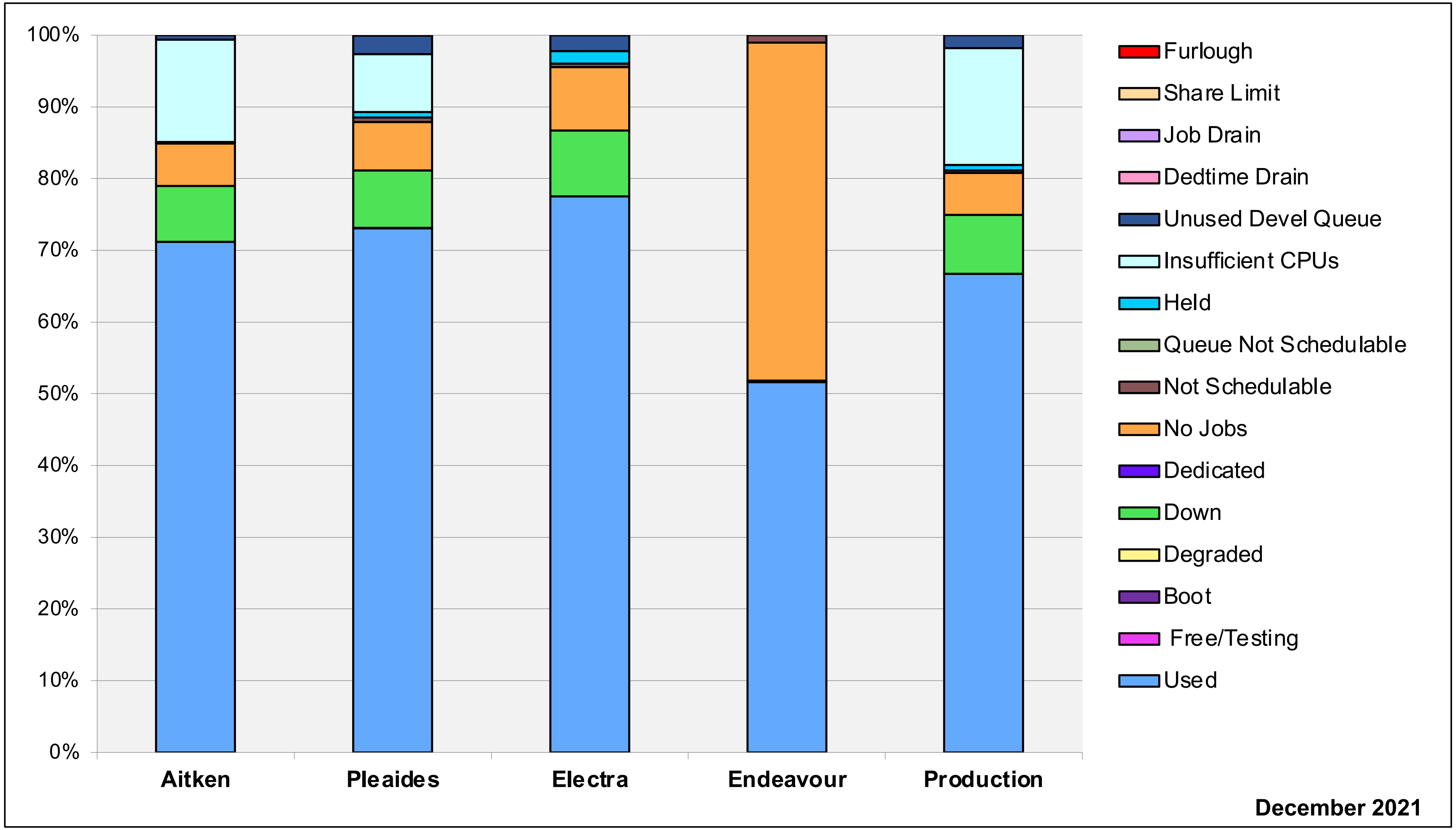
News and Events

- **Scientists Use NASA Data to Predict Corona of Dec. 4 Antarctic Eclipse**, *NASA Goddard*, December 9, 2021—A week in advance, researchers from Predictive Science, Inc. used data from NASA's Solar Dynamics Observatory to predict what the Antarctic eclipse would look like from the ground, utilizing the computing power of the Pleiades supercomputer at the NASA Advanced Supercomputing facility.
https://www.nasa.gov/feature/goddard/2021/scientists-use-nasa-data-to-predict-corona-of-dec-4-antarctic-eclipse
  - **Scientists Use NASA Data to Predict Corona of Dec. 4 Antarctic Eclipse**, *Phys.Org*, December 13, 2021.
https://phys.org/news/2021-12-scientists-nasa-corona-dec-antarctic.html
- **Putting a Bow on it: The NAS Division Wraps Up the Year with SC21**, *NASA Advanced Supercomputing Division*, December 22, 2021—To wrap up the NASA Advanced Supercomputing (NAS) Division's valuable contributions to agency programs, here are 18 research projects led by NAS Division staff and featured at SC21, the International Conference for High-Performance Computing, Networking, Storage, and Analysis—plus, some extra free goodies you can unwrap year-round!
https://www.nas.nasa.gov/pubs/stories/2021/feature_SC21_wrap_Dec_21.html
- **What Computers Do NASA, SpaceX And Blue Origin Use?** *CCL Computing,* December 29, 2021—A look at the technology used in space exploration, including the Pleiades supercomputer, the NASA Advanced Supercomputing (NAS) facility environment, and some history on NAS's leadership in HPC.
https://www.cclonline.com/article/2039/Guide/CCL-Gaming-PCs/What-Computers-Do-NASA-SpaceX-And-Blue-Origin-Use-/

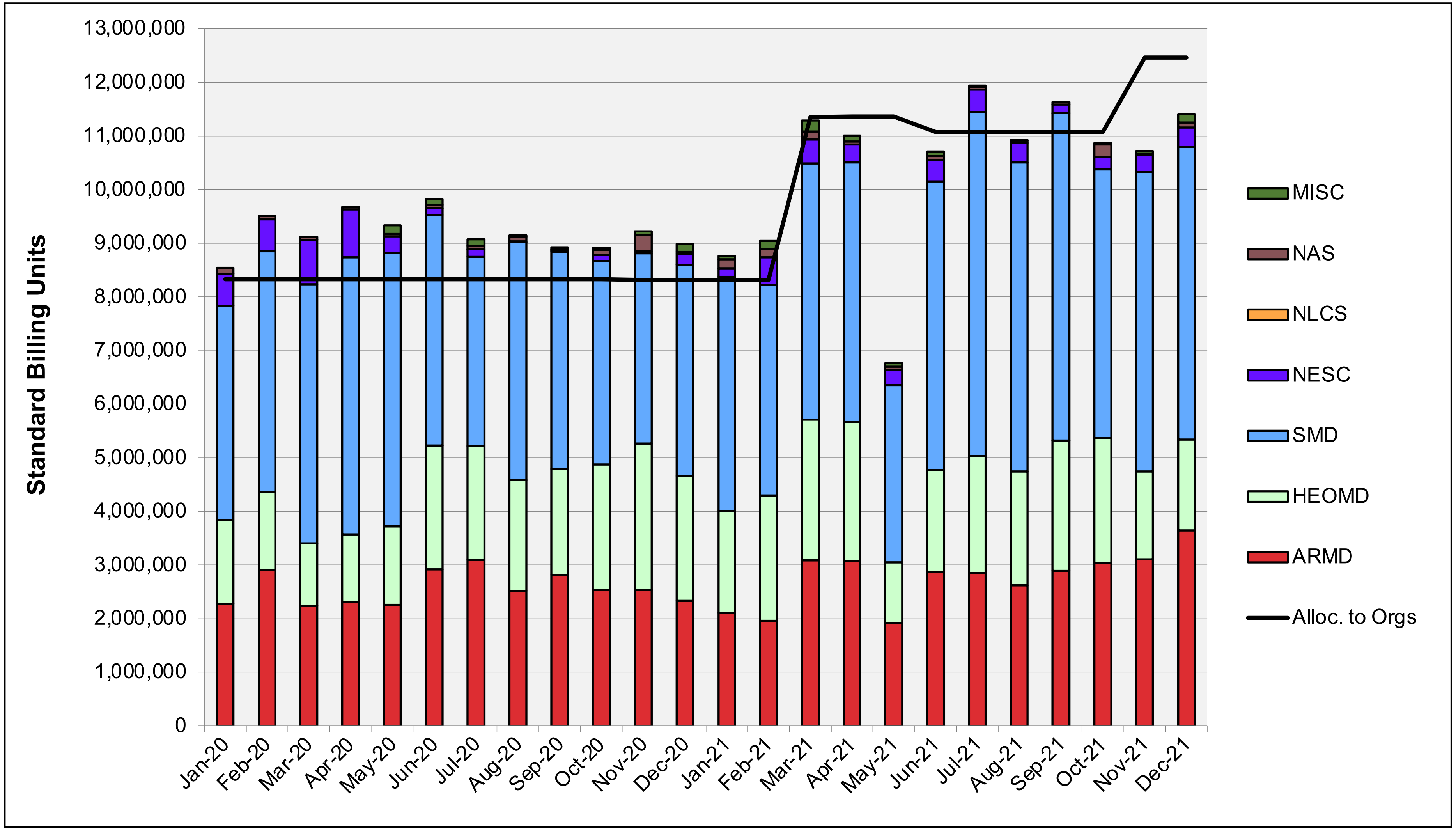
News and Events: Social Media

- **Coverage of NAS Stories**
  - December 4th Total Eclipse Prediction:
    - NAS: Twitter 3 retweets, 6 likes.
    - NASA Supercomputing: Twitter 5 retweets, 19 likes; Facebook 305 users reached, 33 engagements, 19 likes, 3 shares.
  - Dimitris Menemenlis, ECCO presentation/SC21:
    - NAS: Twitter 5 retweets, 17 likes.
  - NAS 2021 Recap:
    - NAS: Twitter 9 retweets, 23 likes.

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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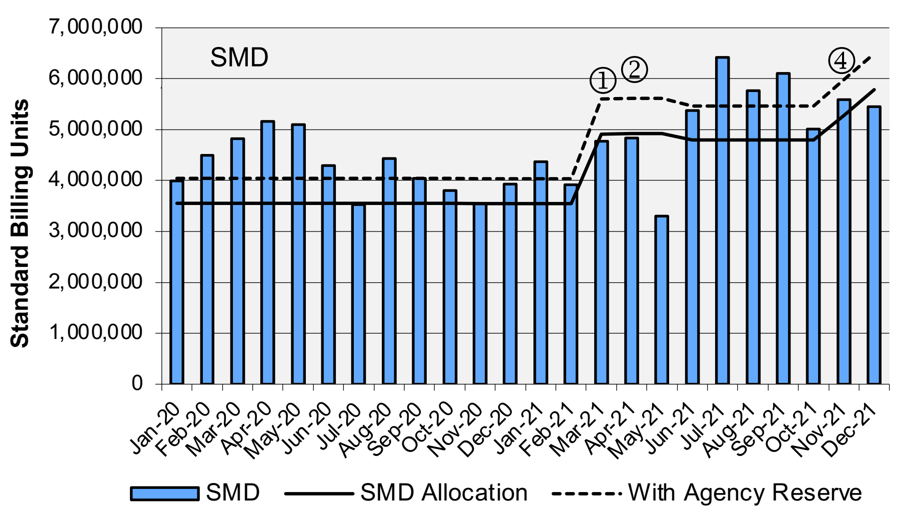
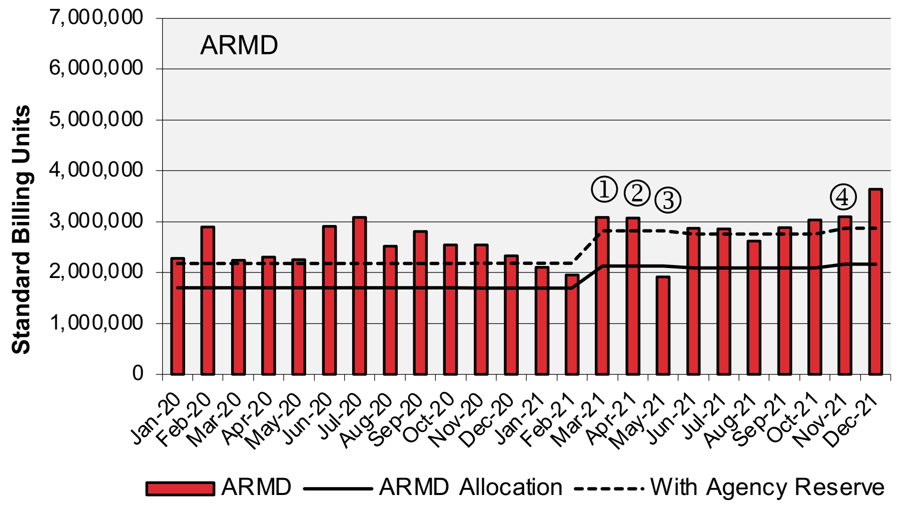
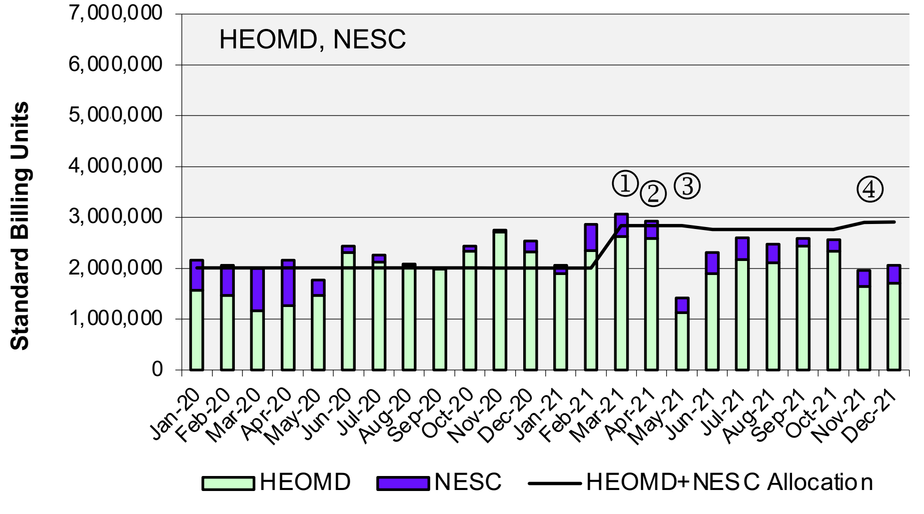






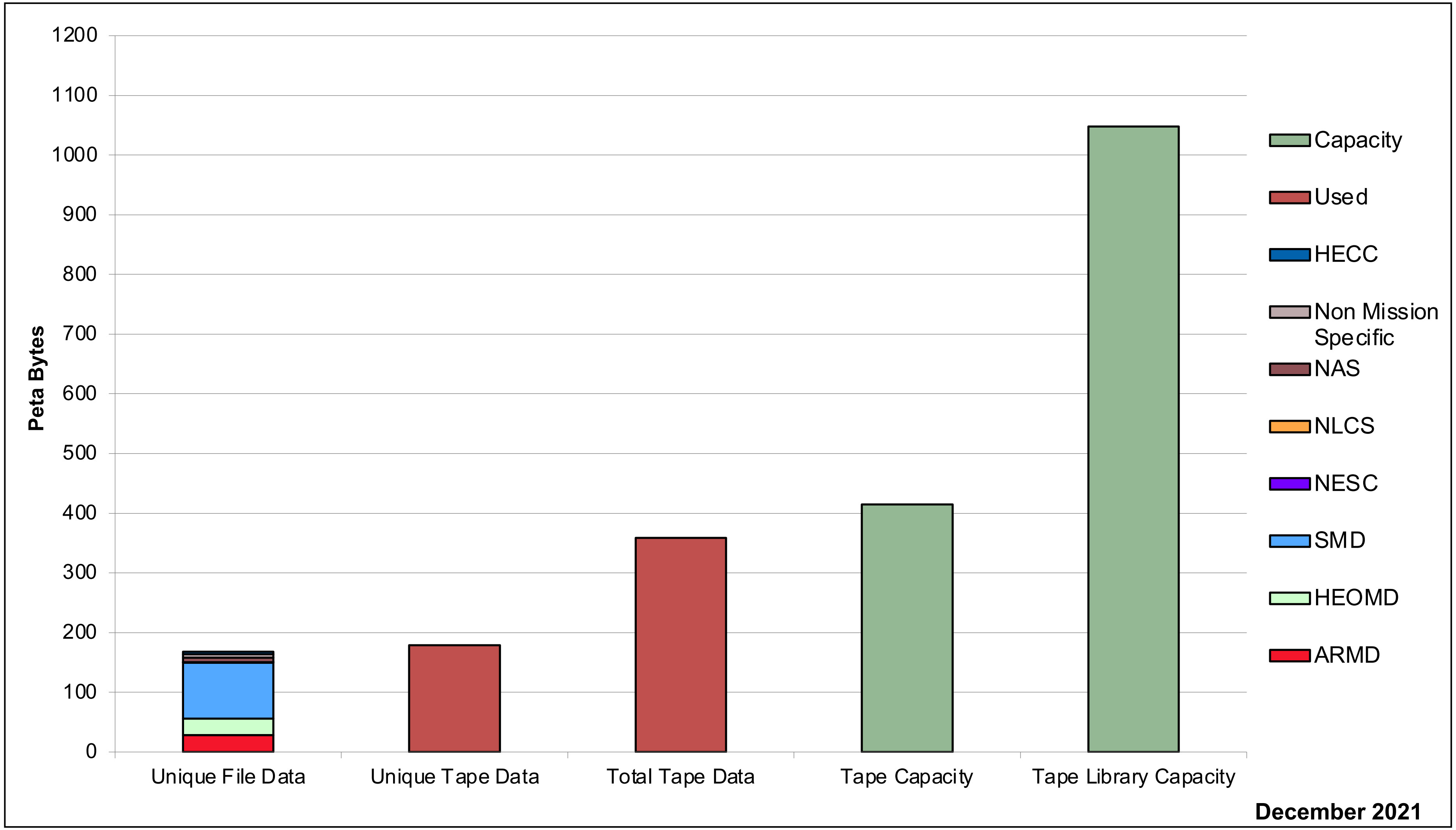
① 8 Rome Apollo racks introduced into Aitken

② Endeavour replaced with new hardware

③ Merope retired

④ 4 Rome Apollo Racks added to Aitken

Tape Archive Status



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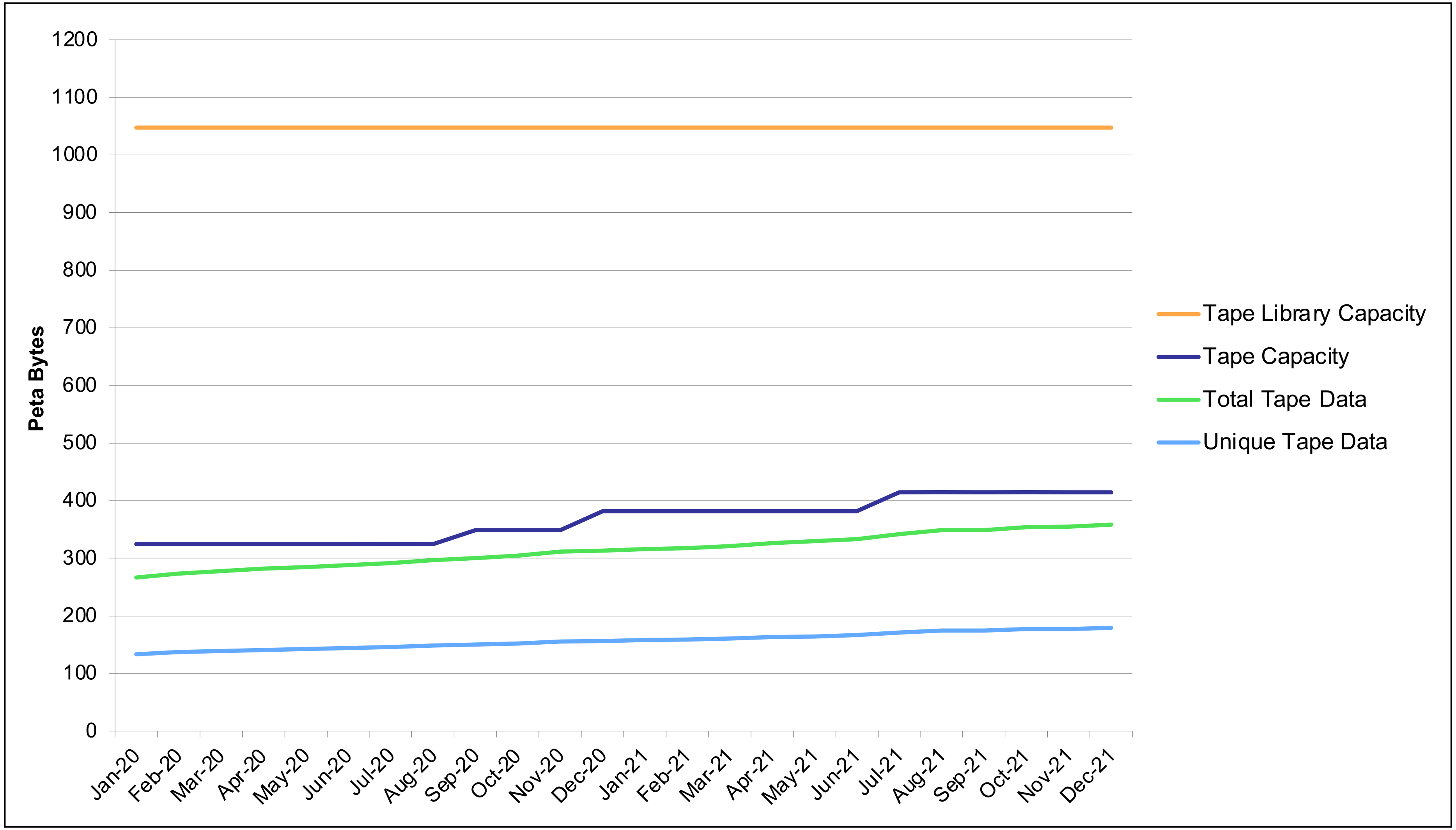
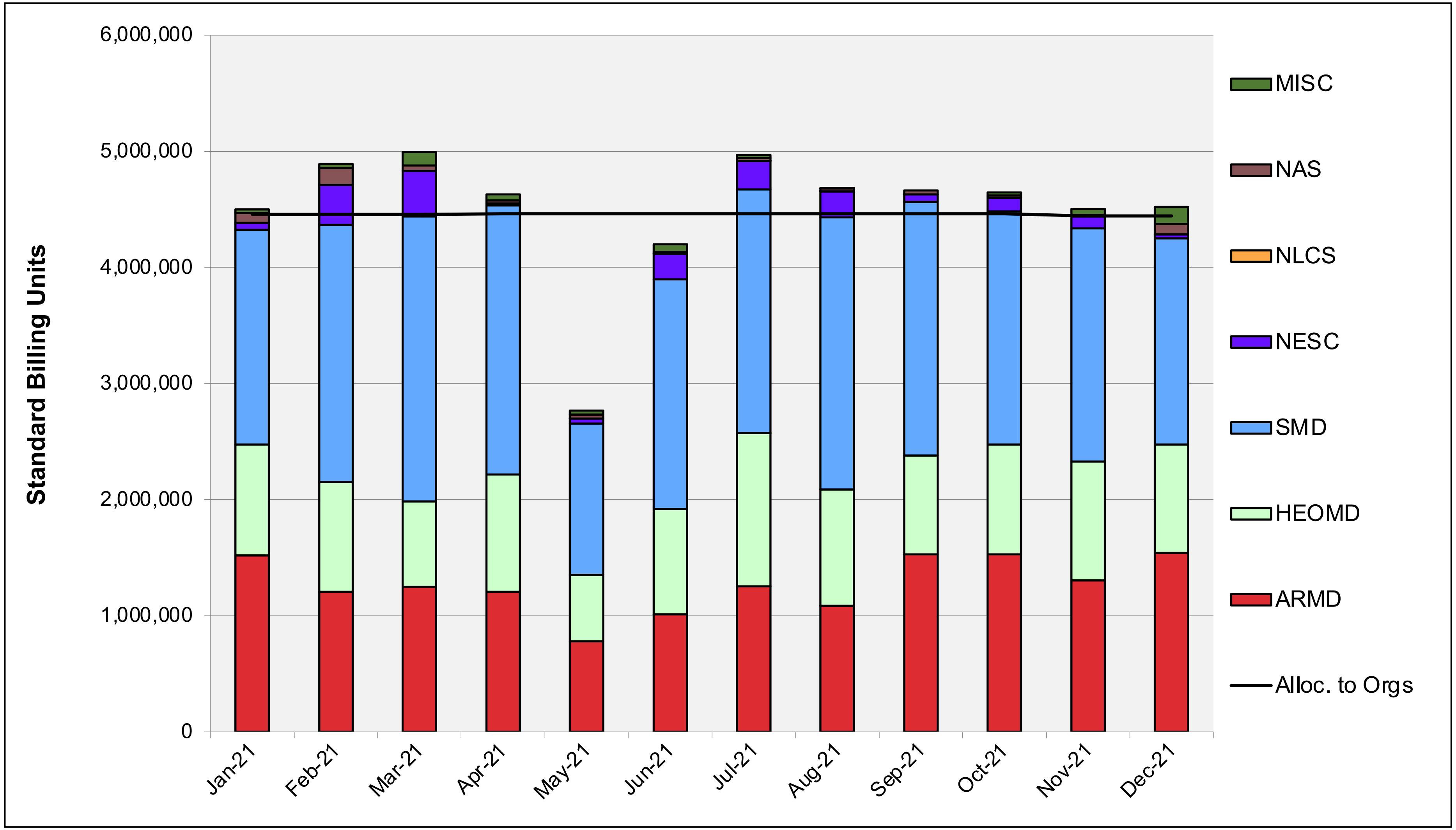
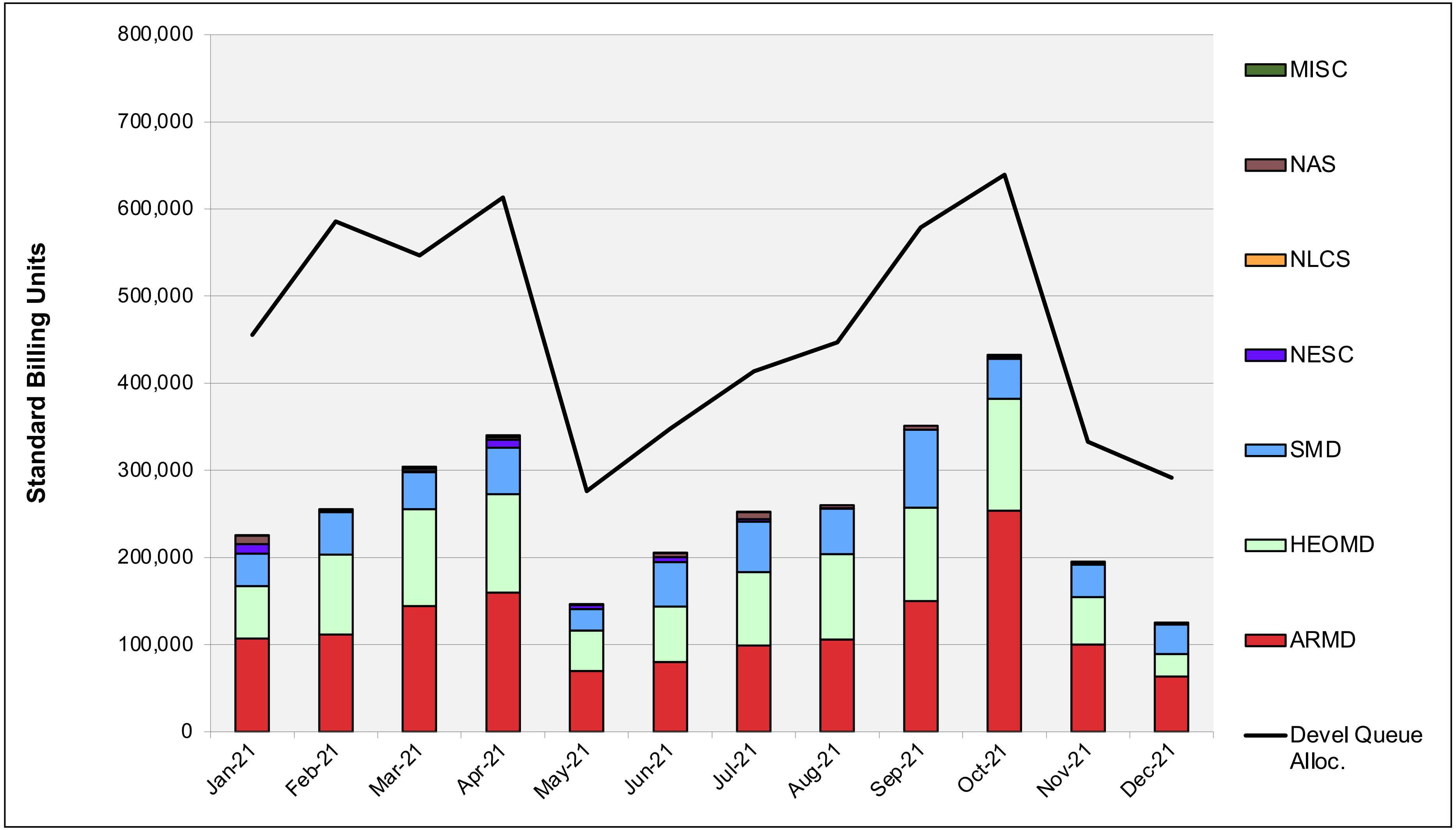


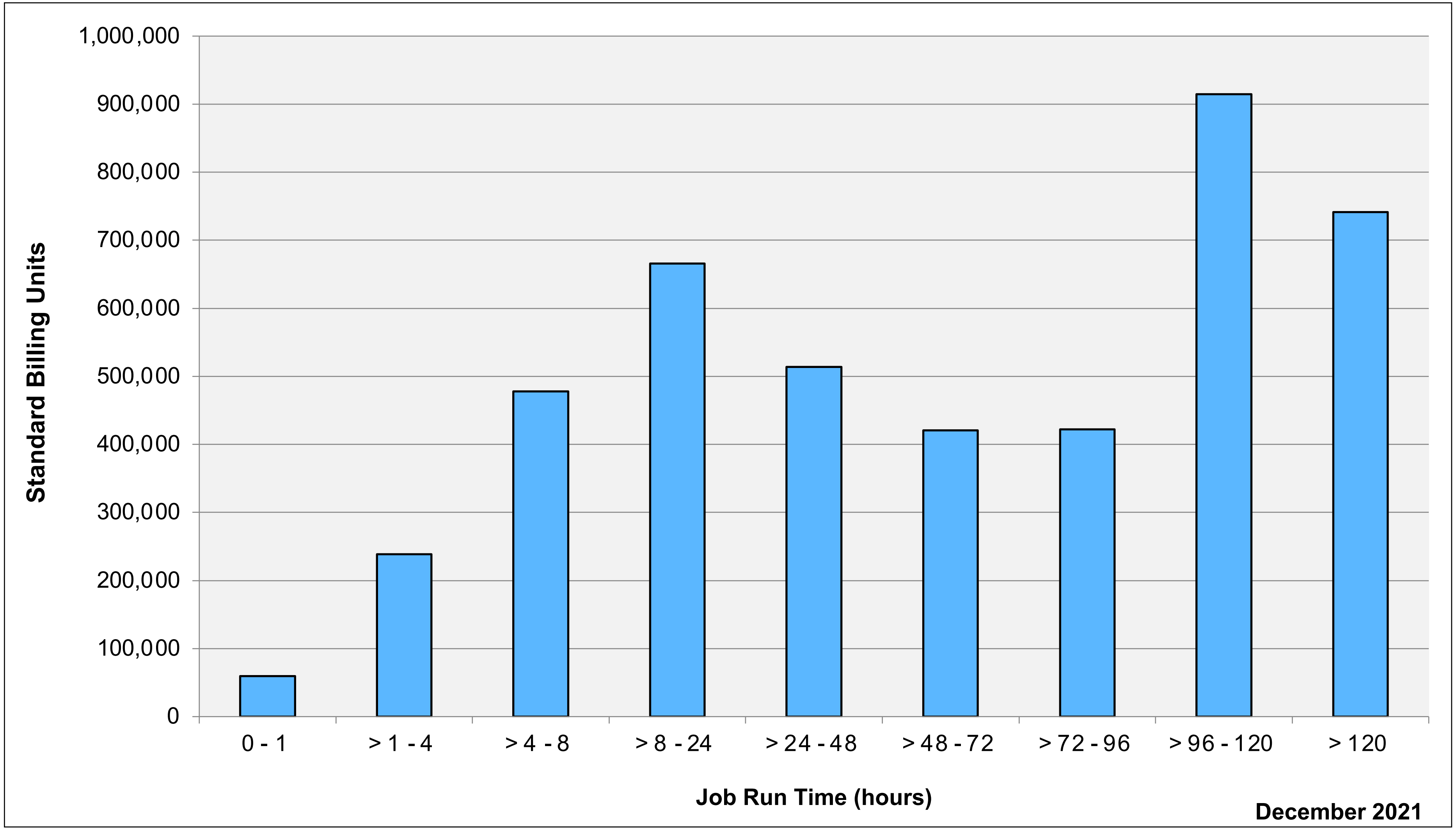
Pleiades: SBUs Reported, Normalized to 30-Day Month



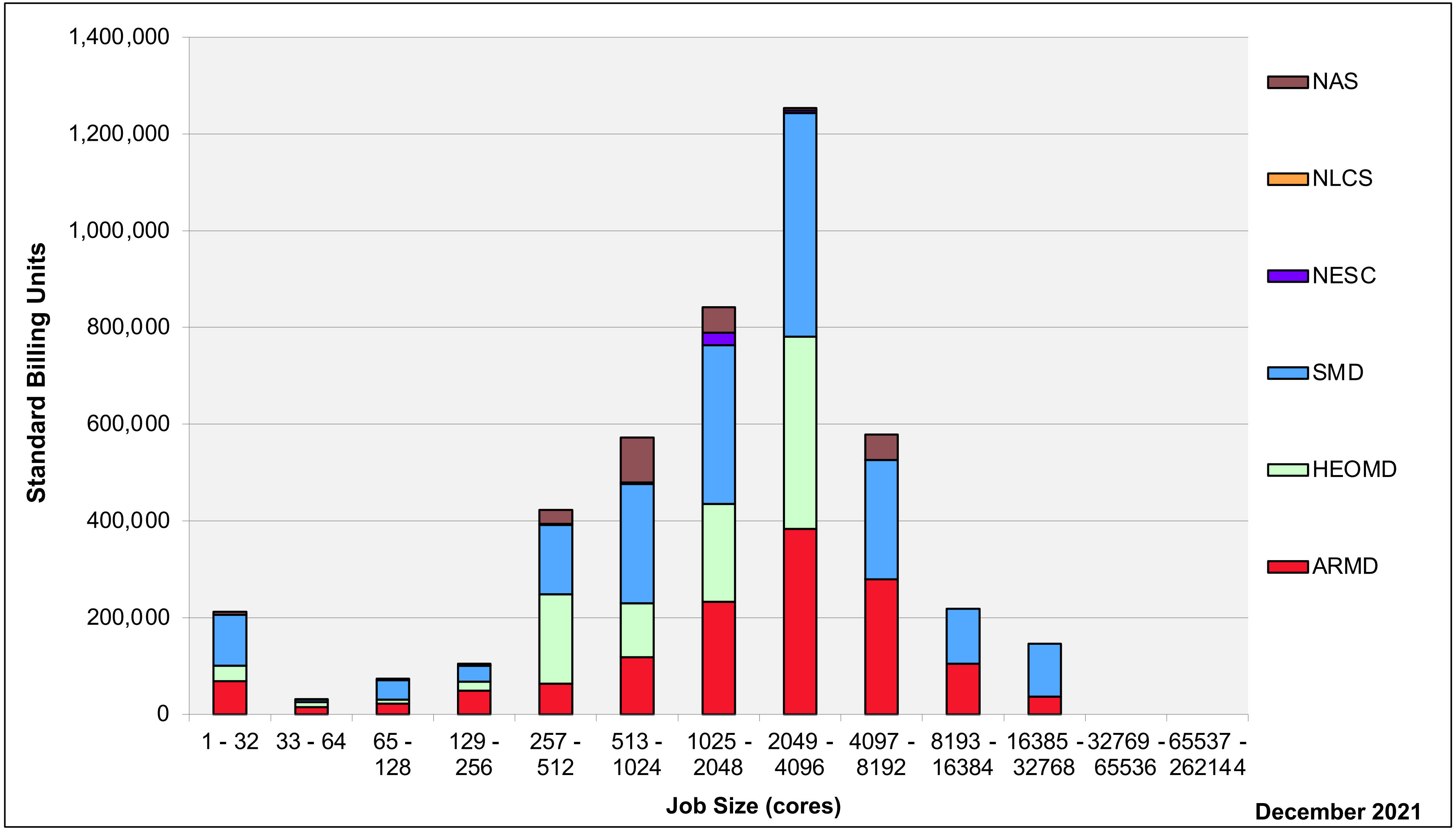
Pleiades: Devel Queue Utilization



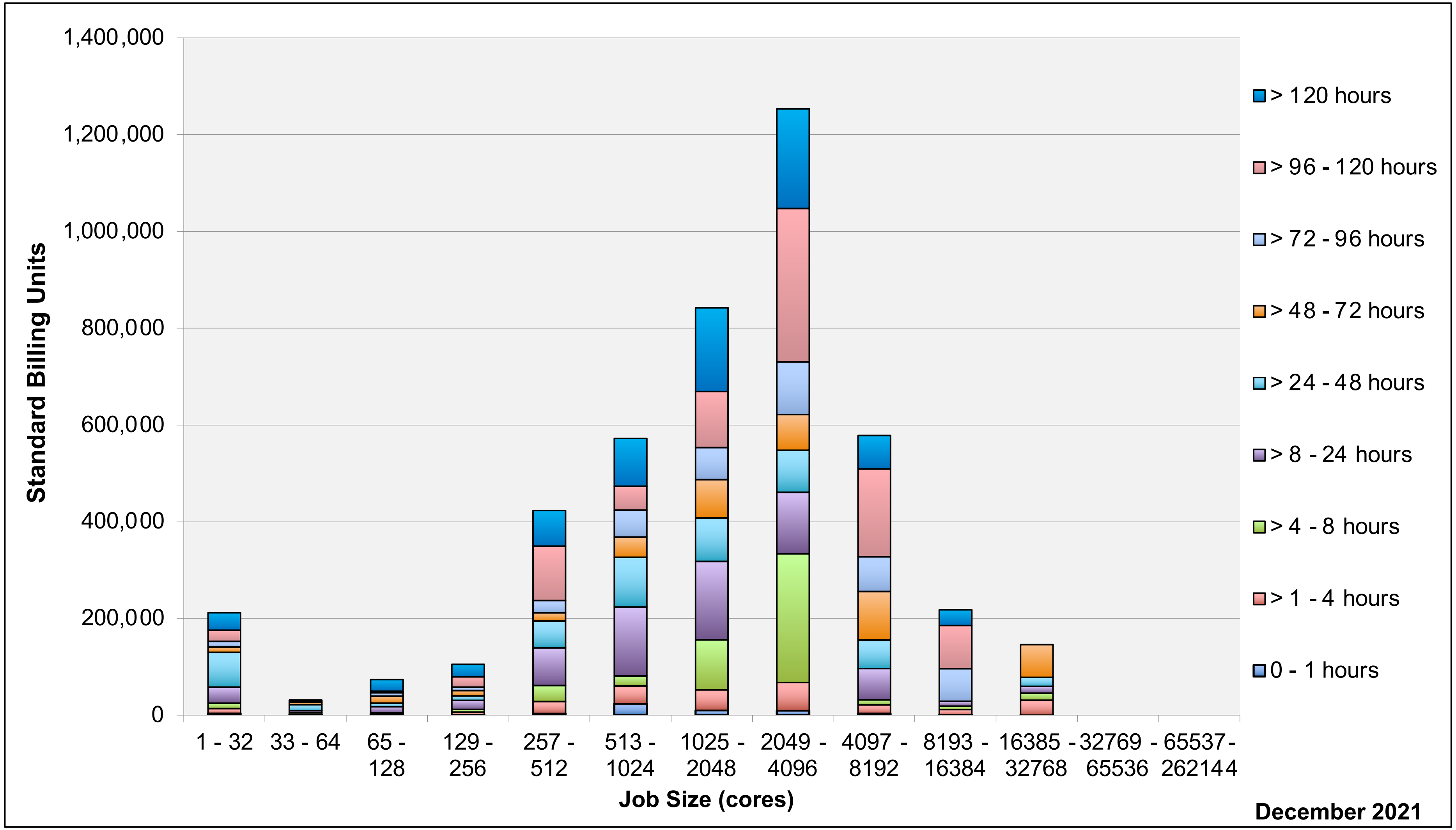
Pleiades: Monthly Utilization by Job Length



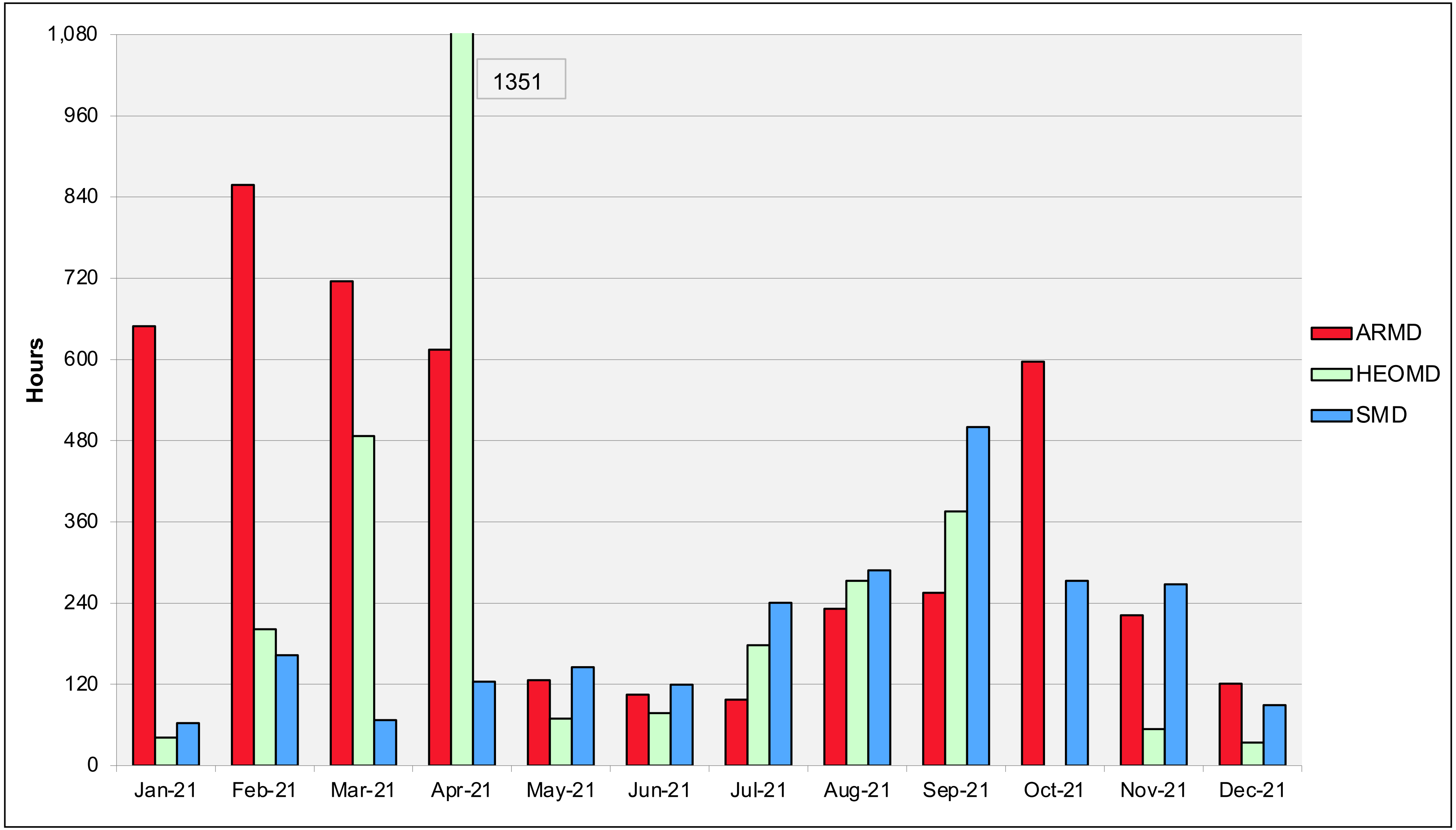
Pleiades: Monthly Utilization by Job Size



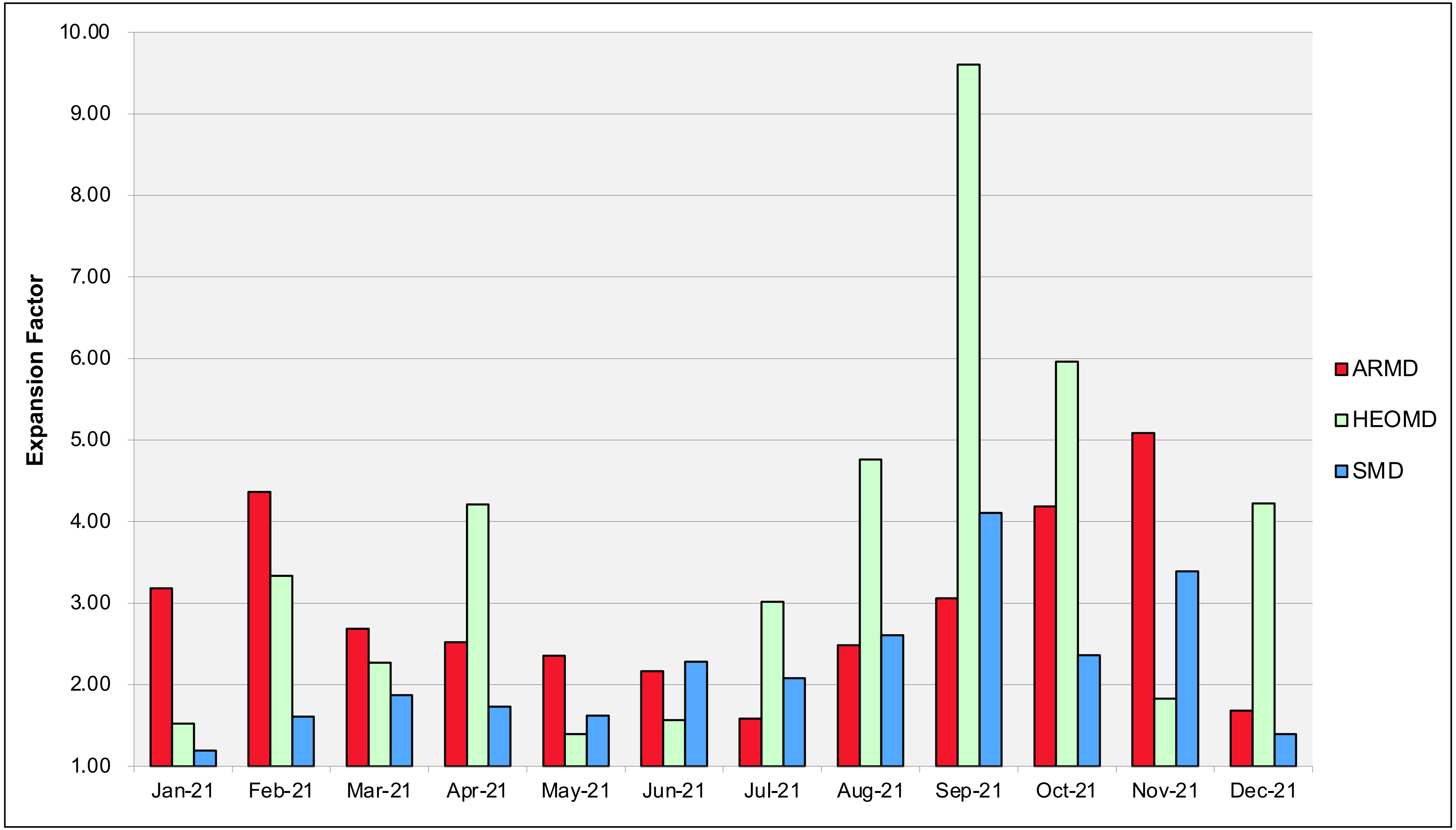
Pleiades: Monthly Utilization by Size and Length



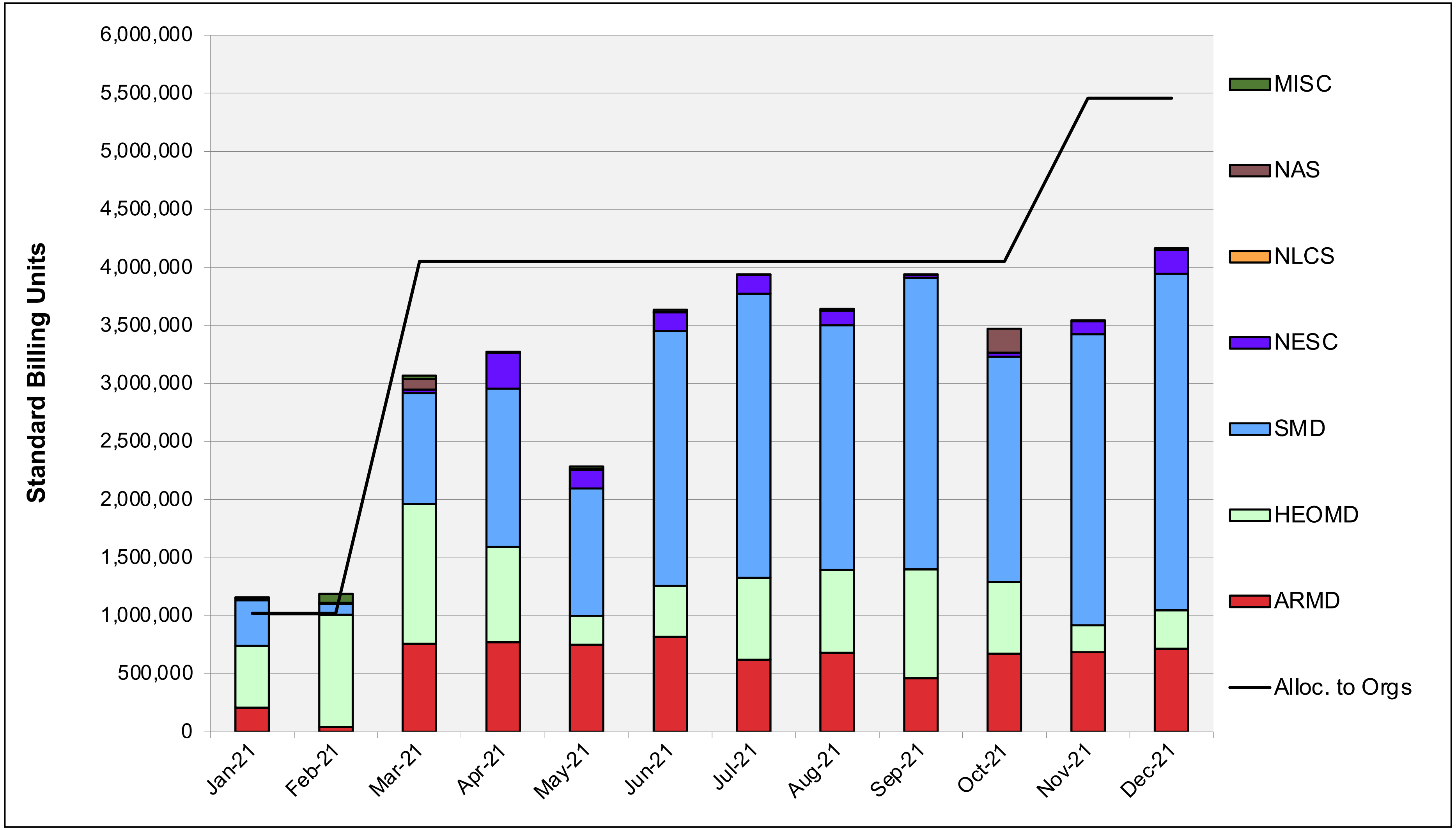
Pleiades: Average Time to Clear All Jobs



Pleiades: Average Expansion Factor



Aitken: SBUs Reported, Normalized to 30-Day Month



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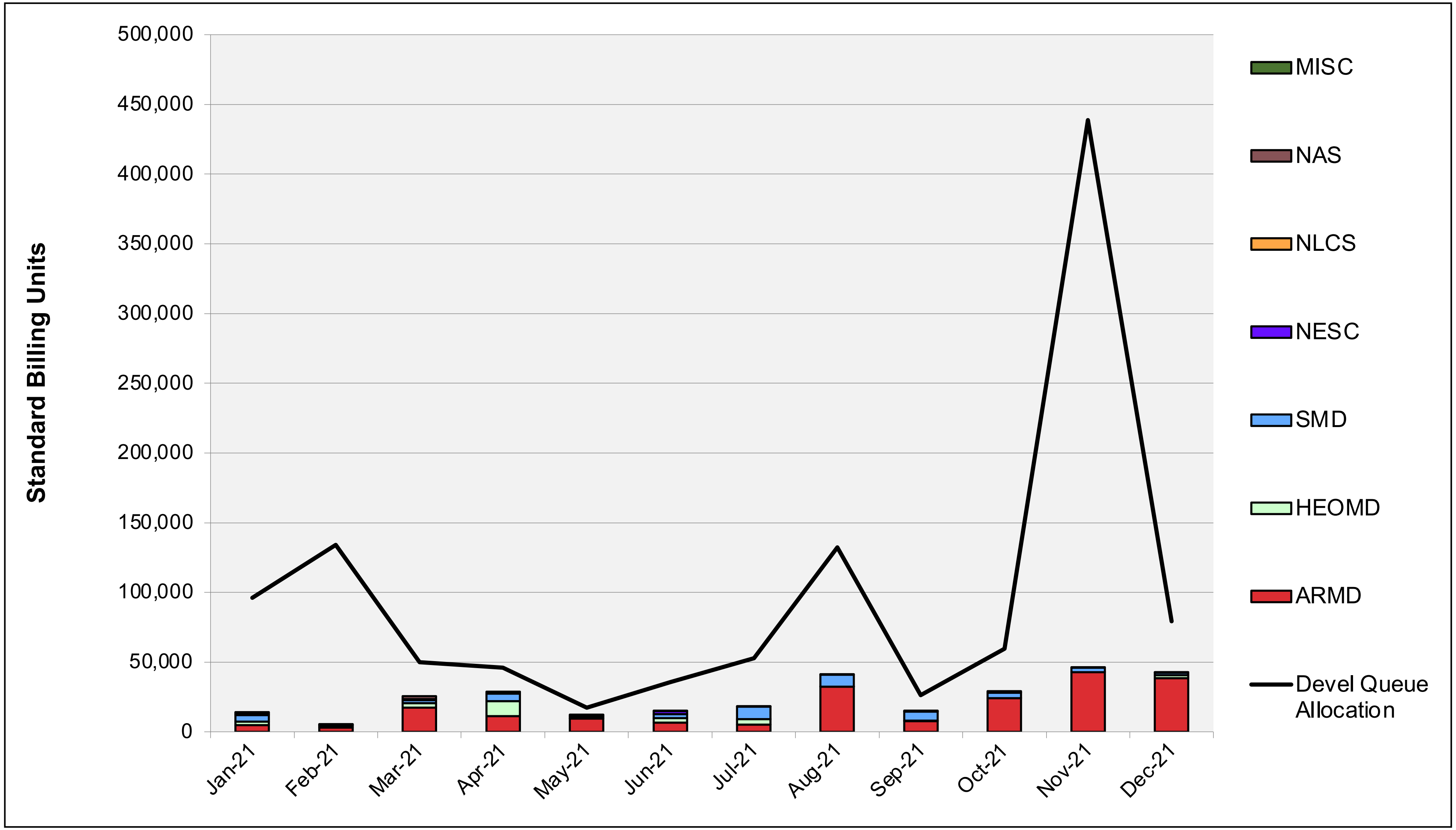
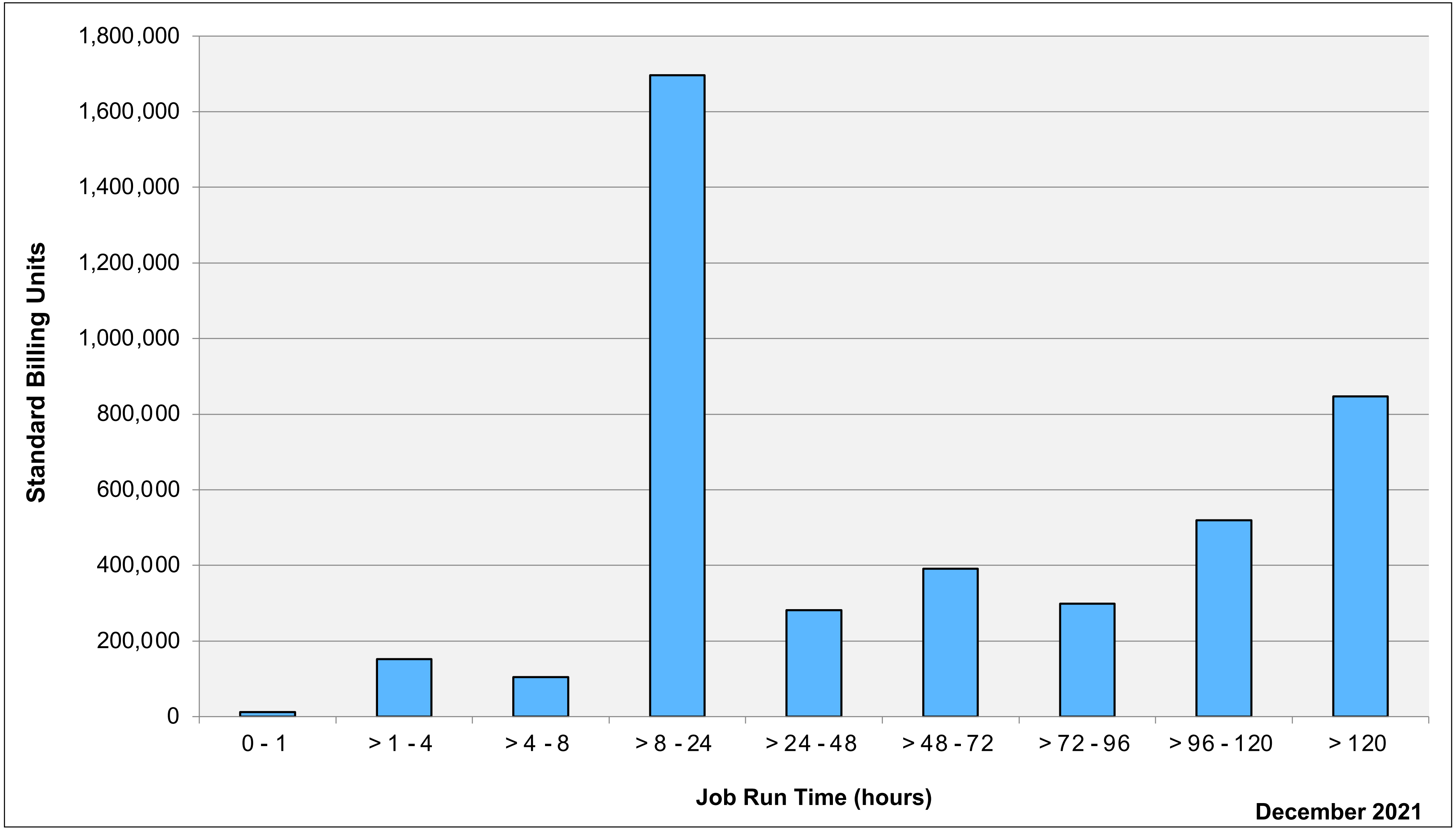


Aitken: Monthly Utilization by Job Length



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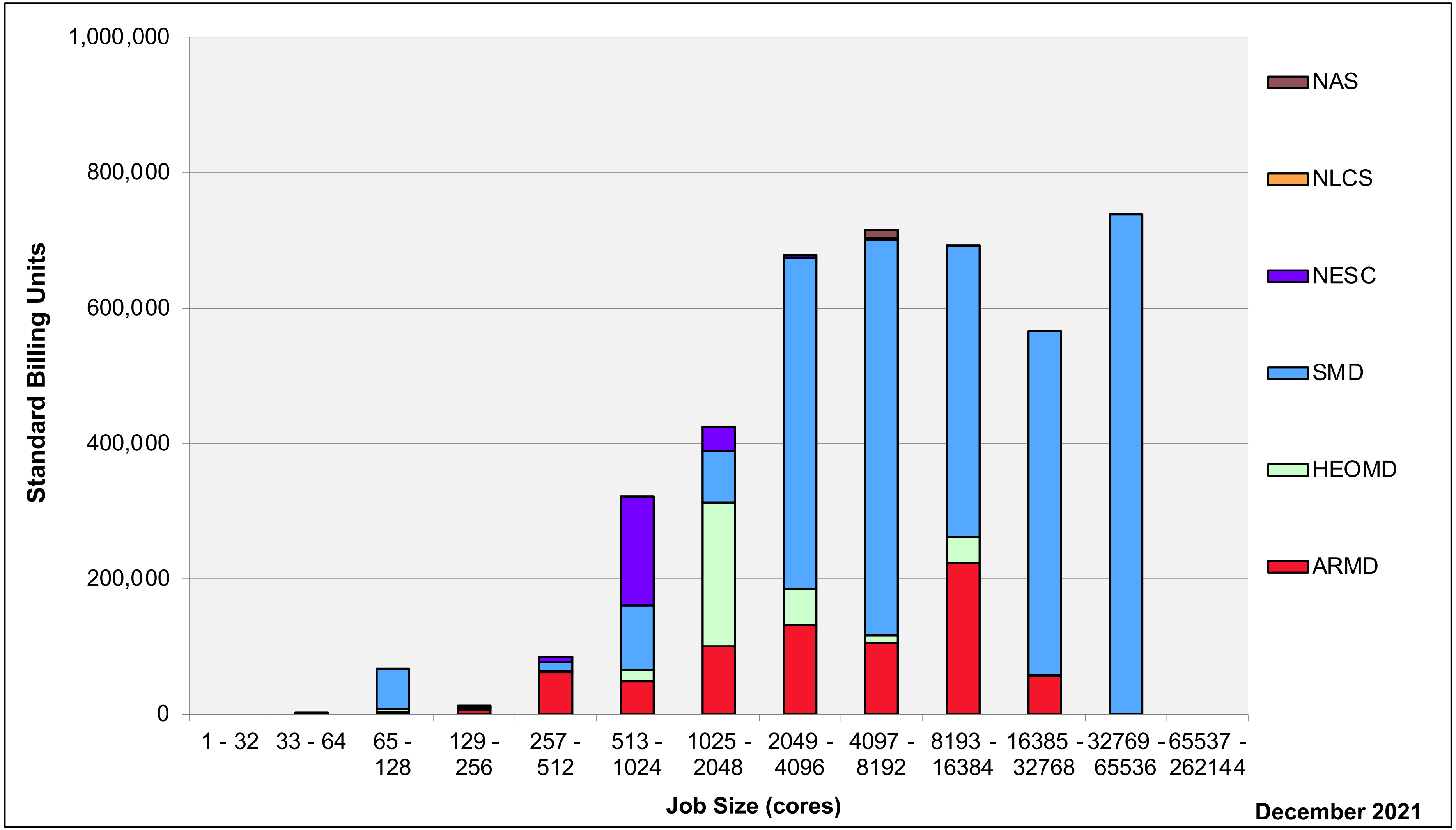
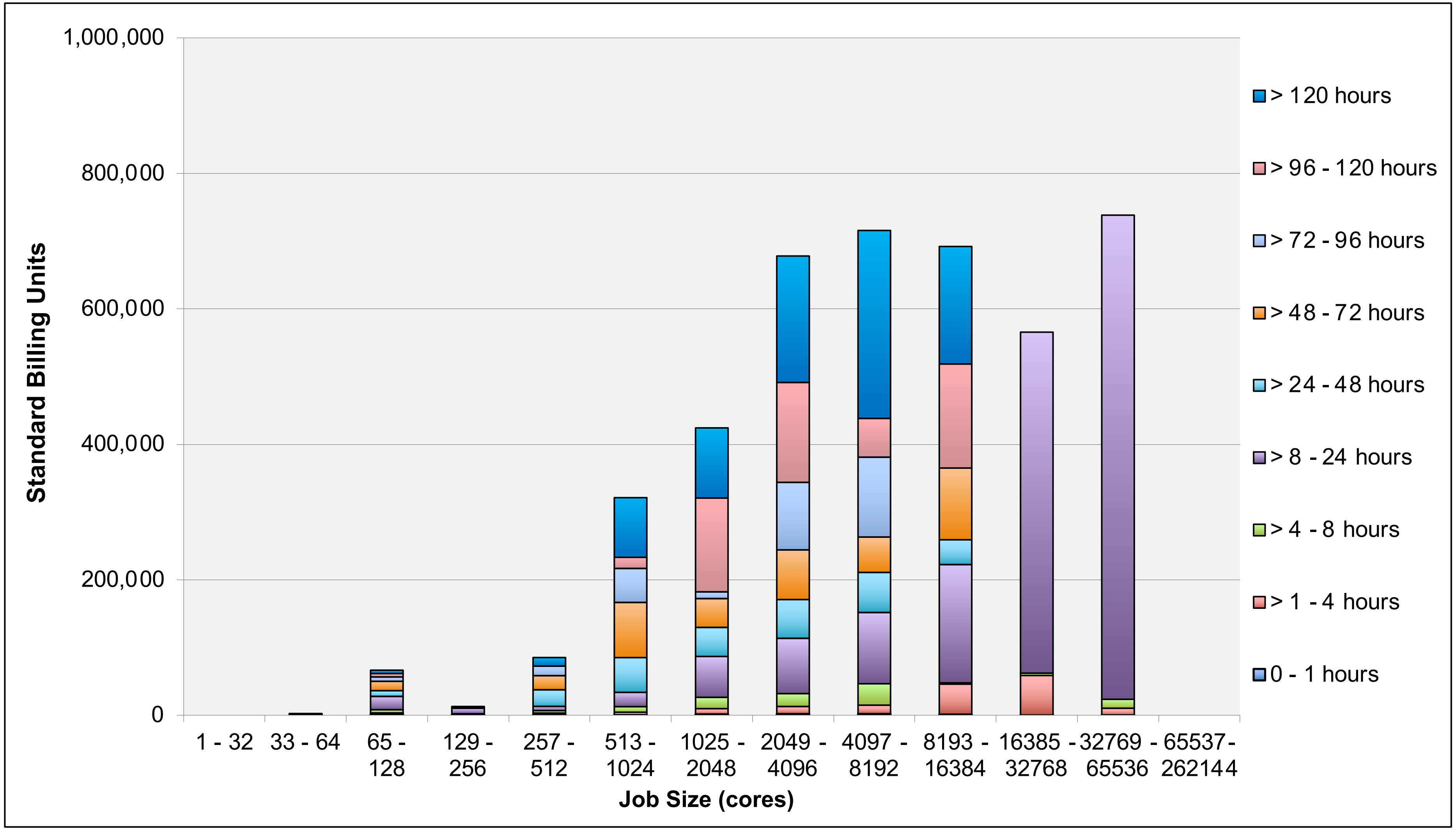
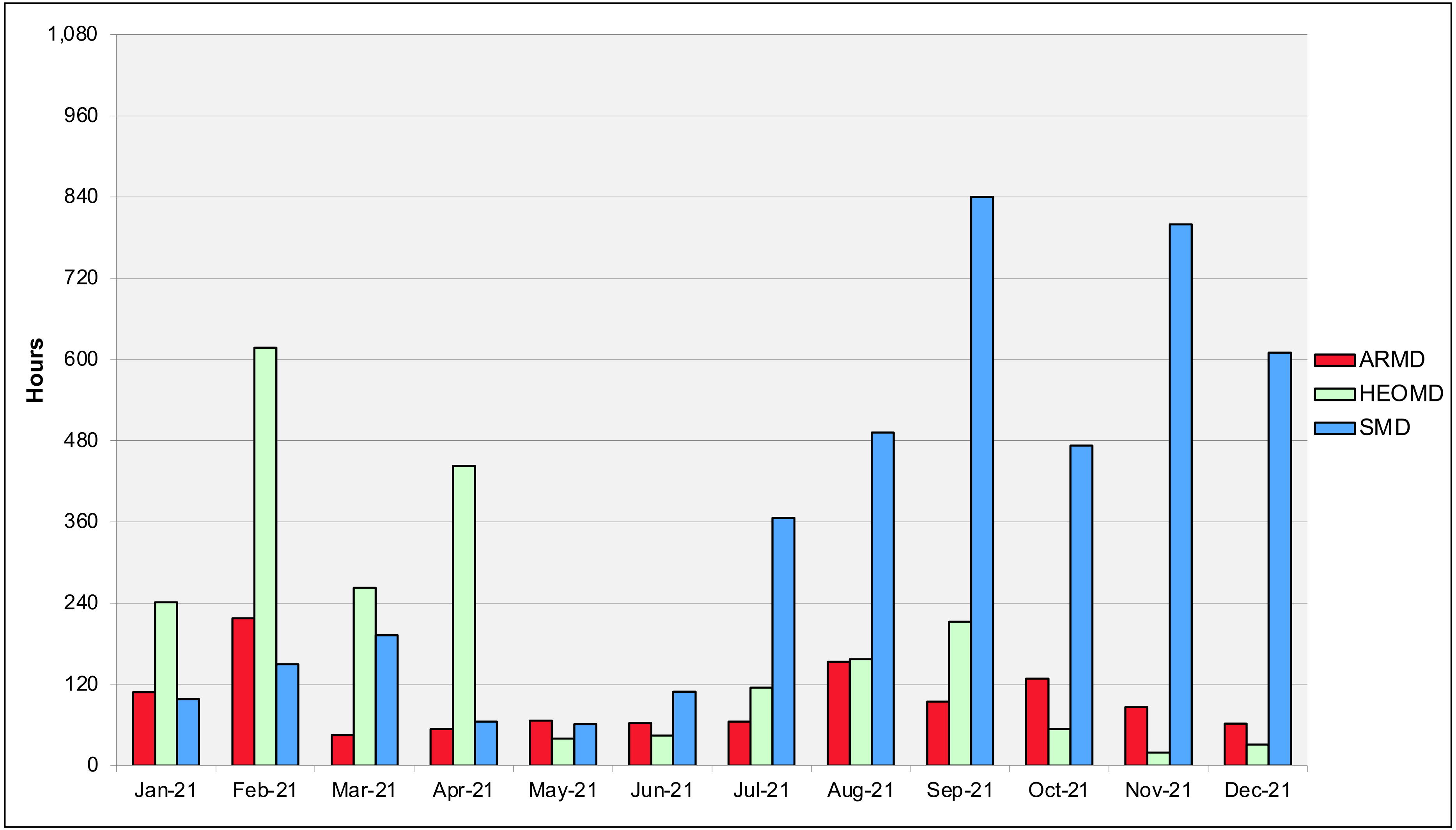


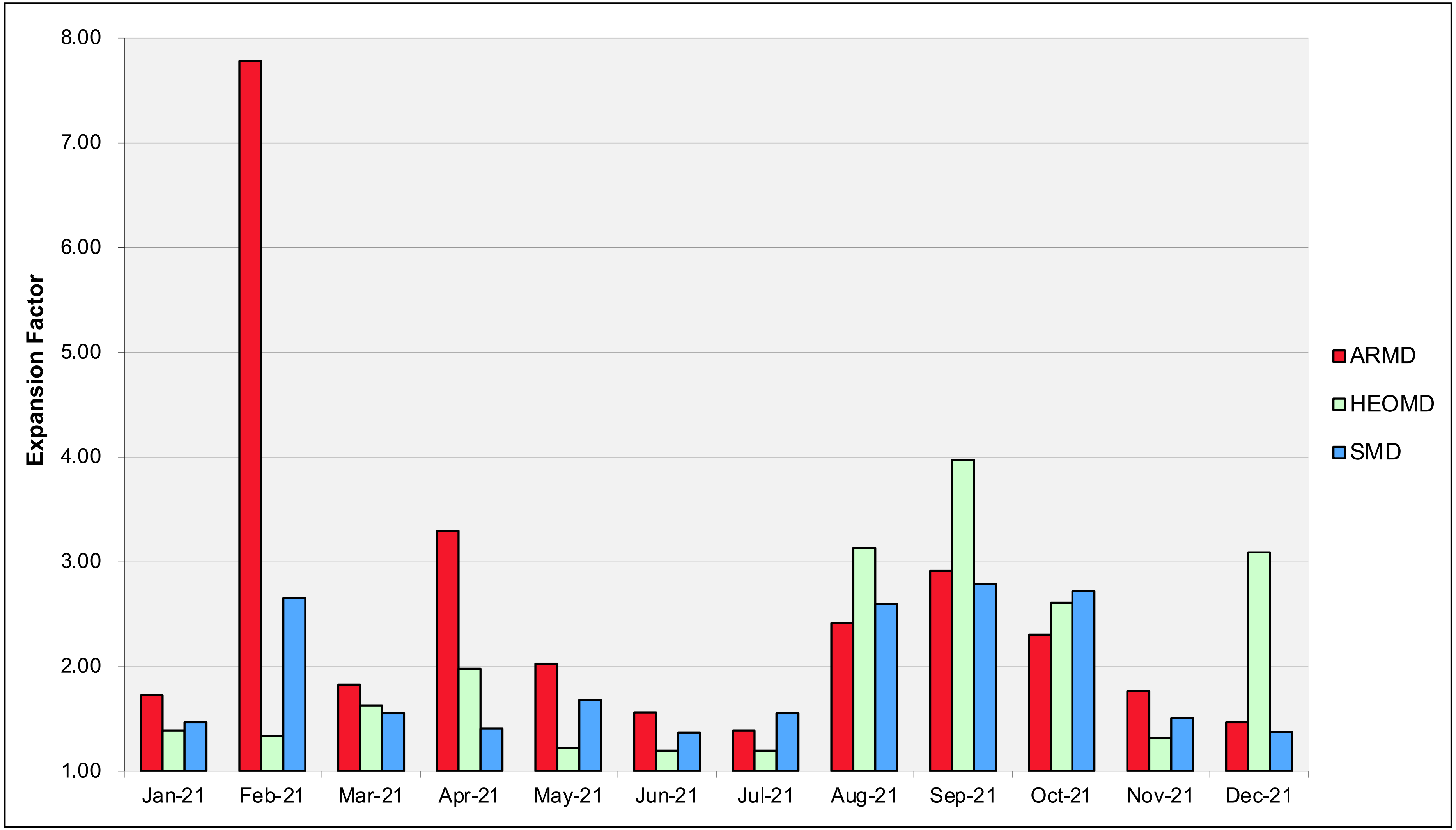
Aitken: Monthly Utilization by Size and Length



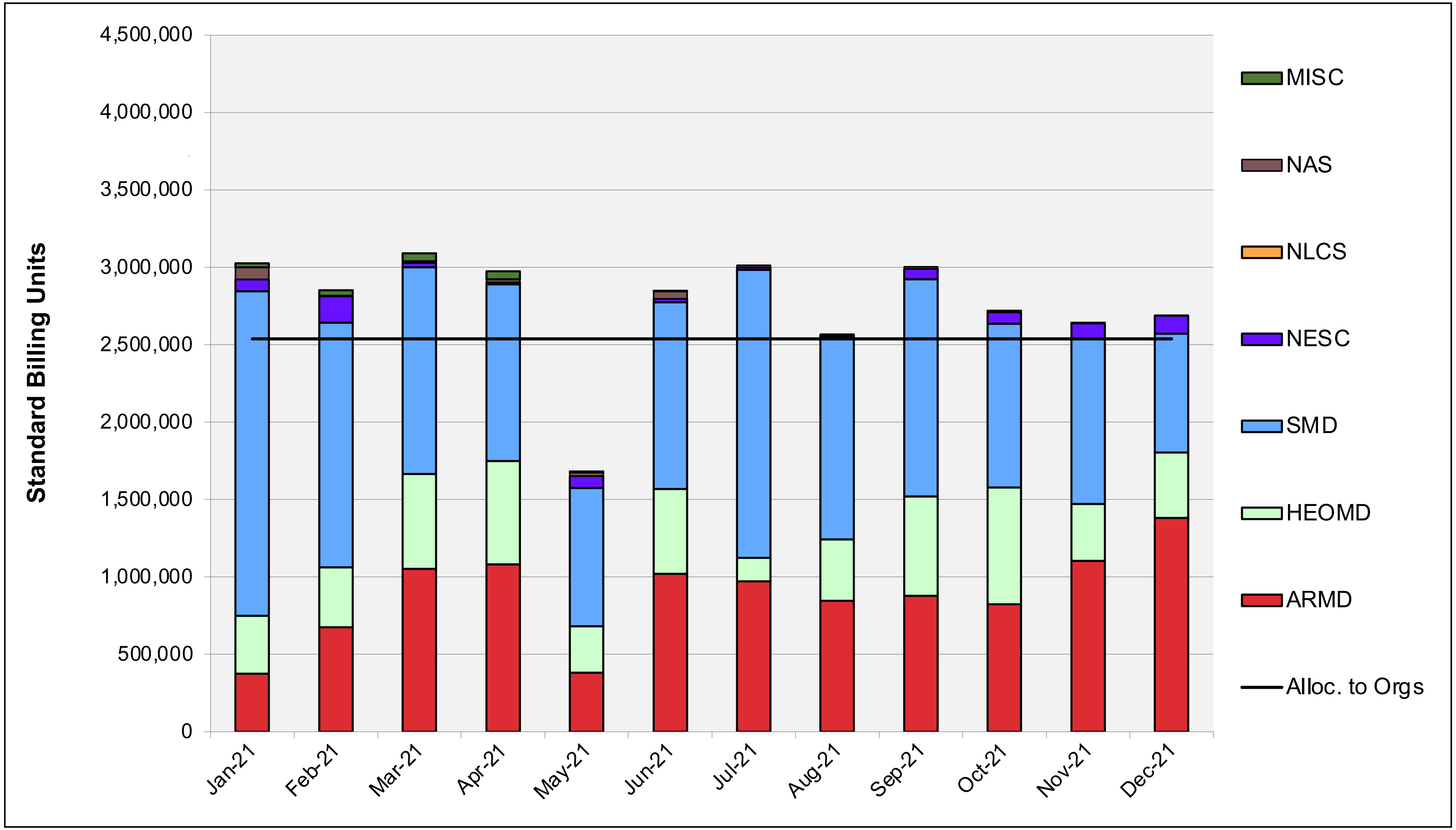
Aitken: Average Time to Clear All Jobs



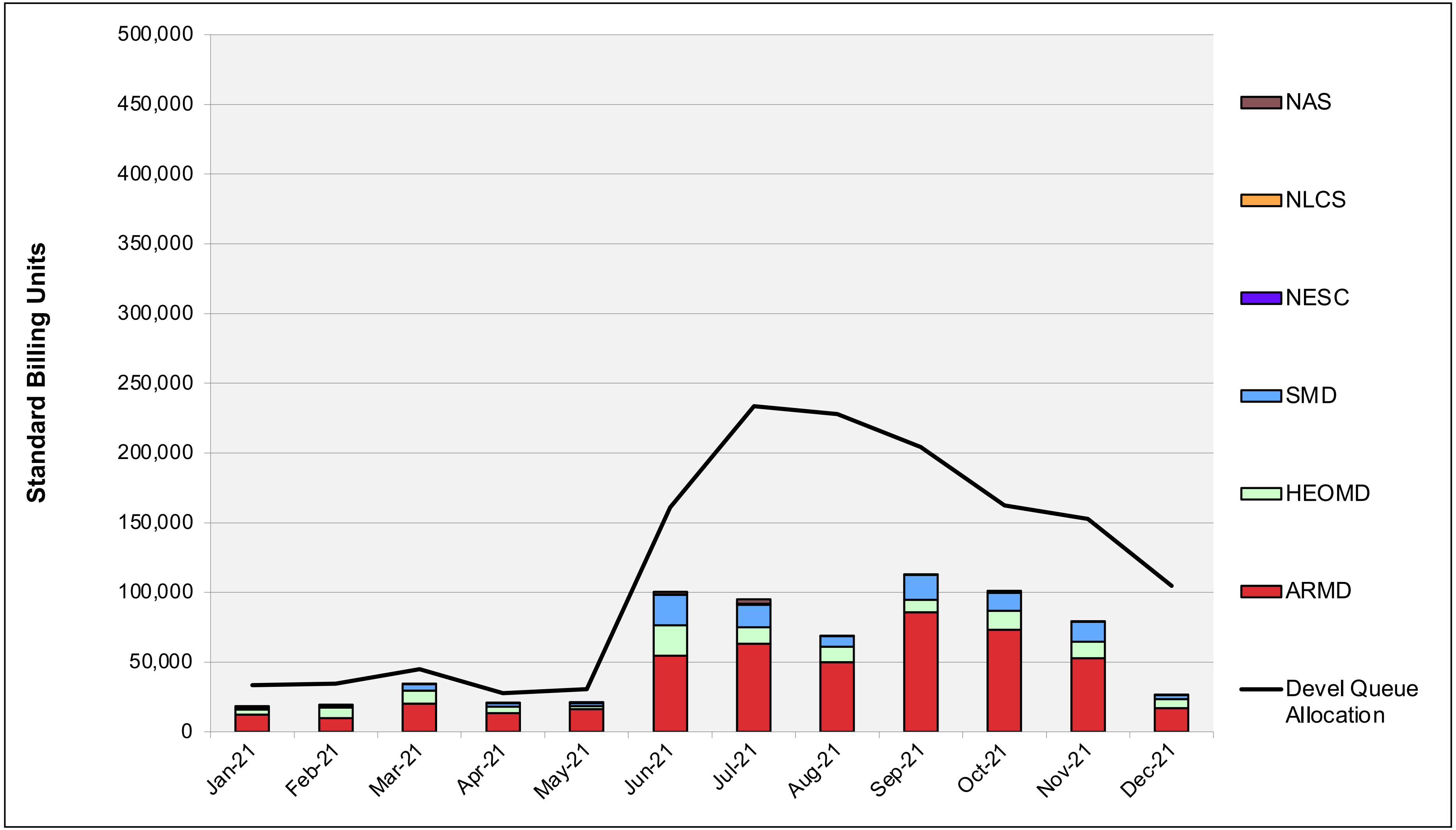
Aitken: Average Expansion Factor



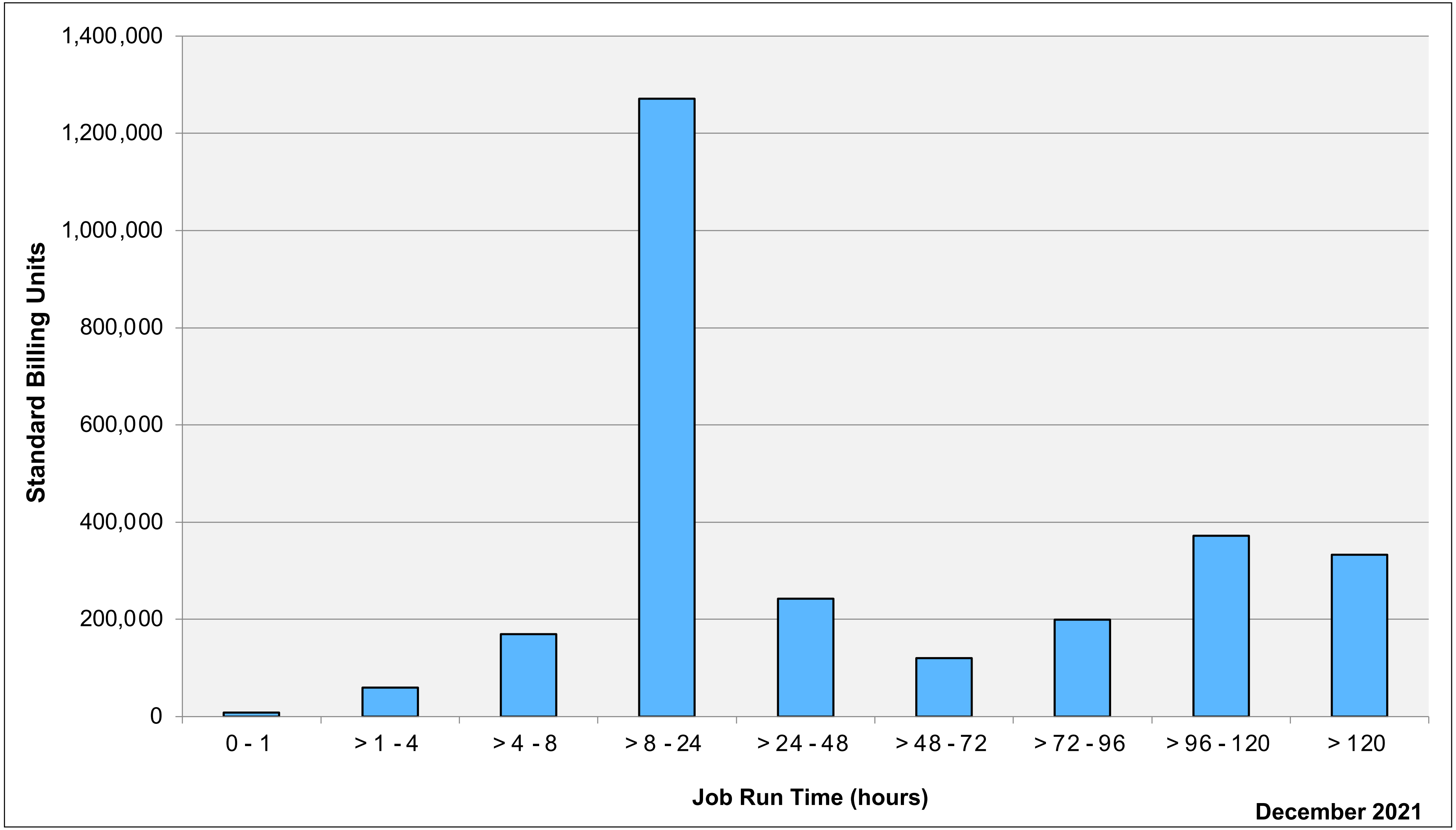
Electra: SBUs Reported, Normalized to 30-Day Month



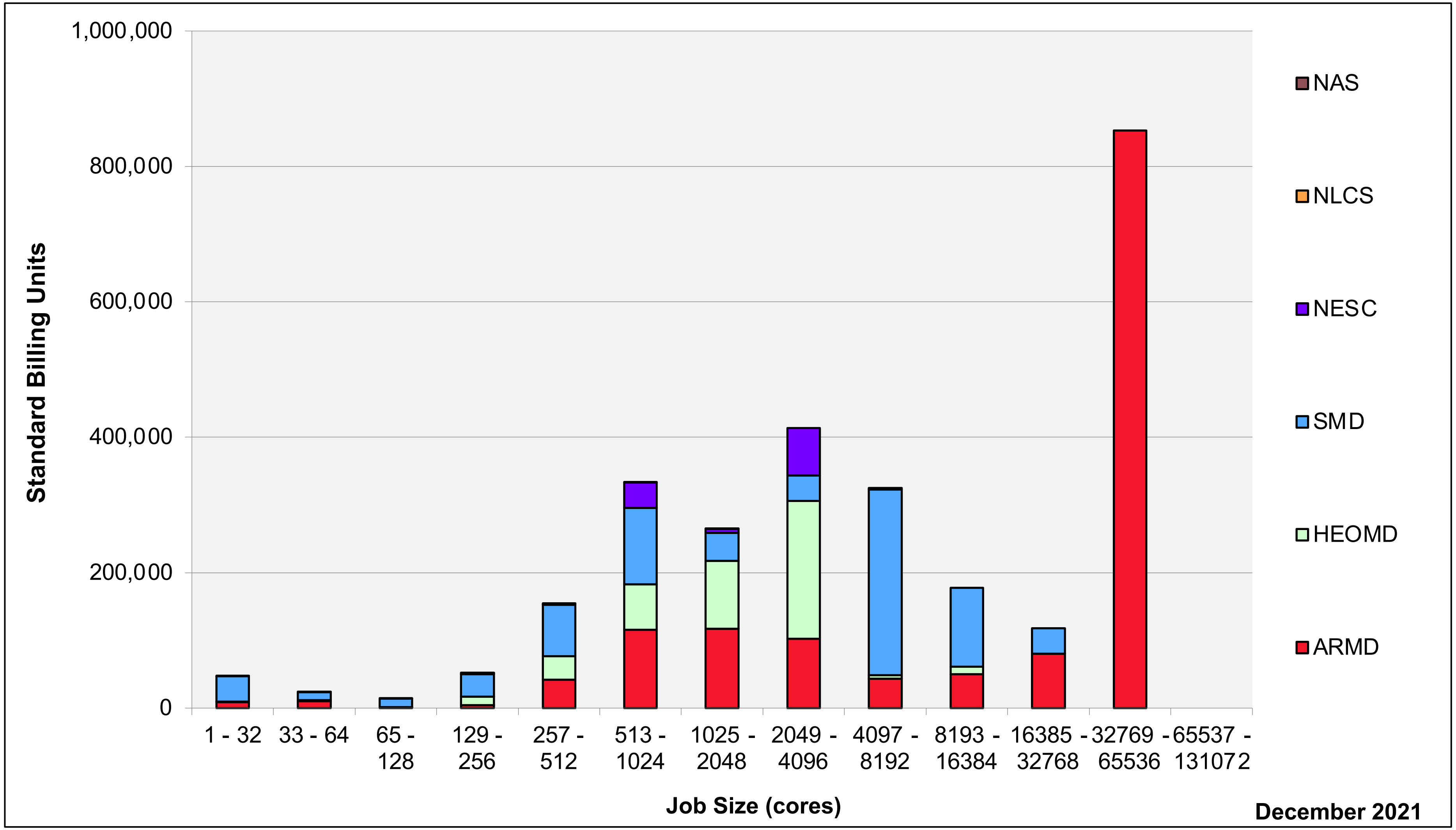
Electra: Devel Queue Utilization



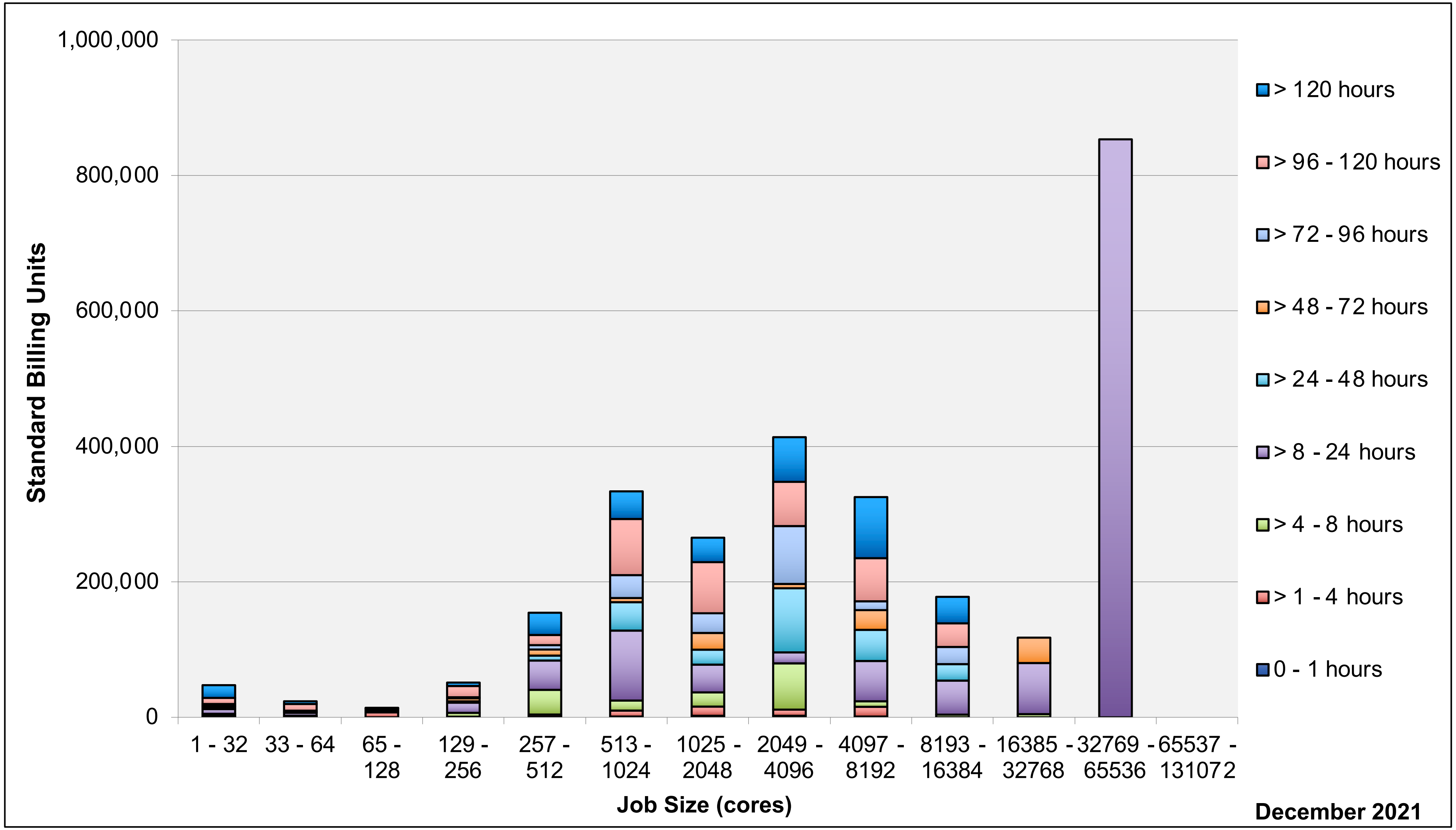
Electra: Monthly Utilization by Job Length



Electra: Monthly Utilization by Job Size



Electra: Monthly Utilization by Size and Length



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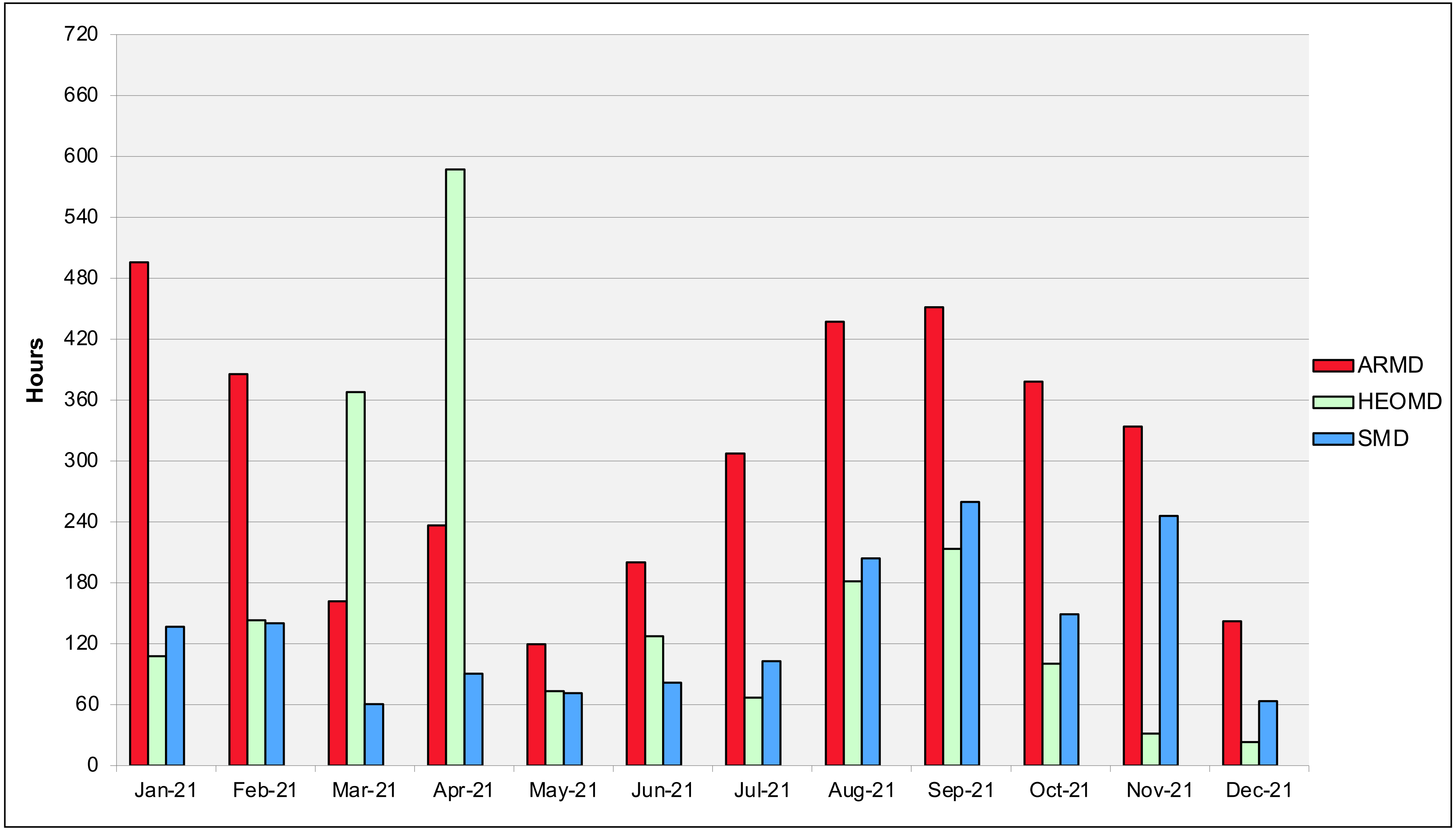

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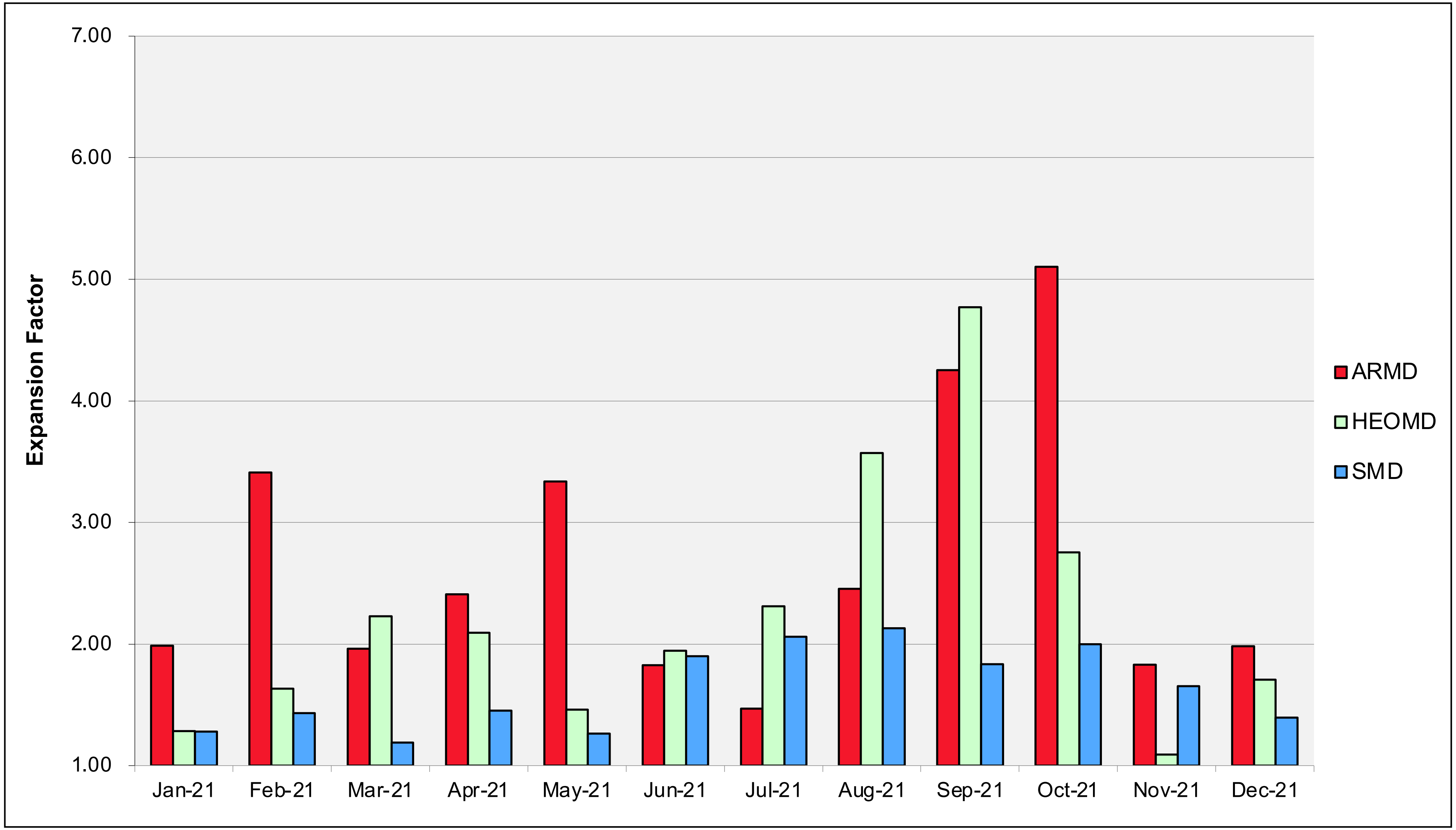
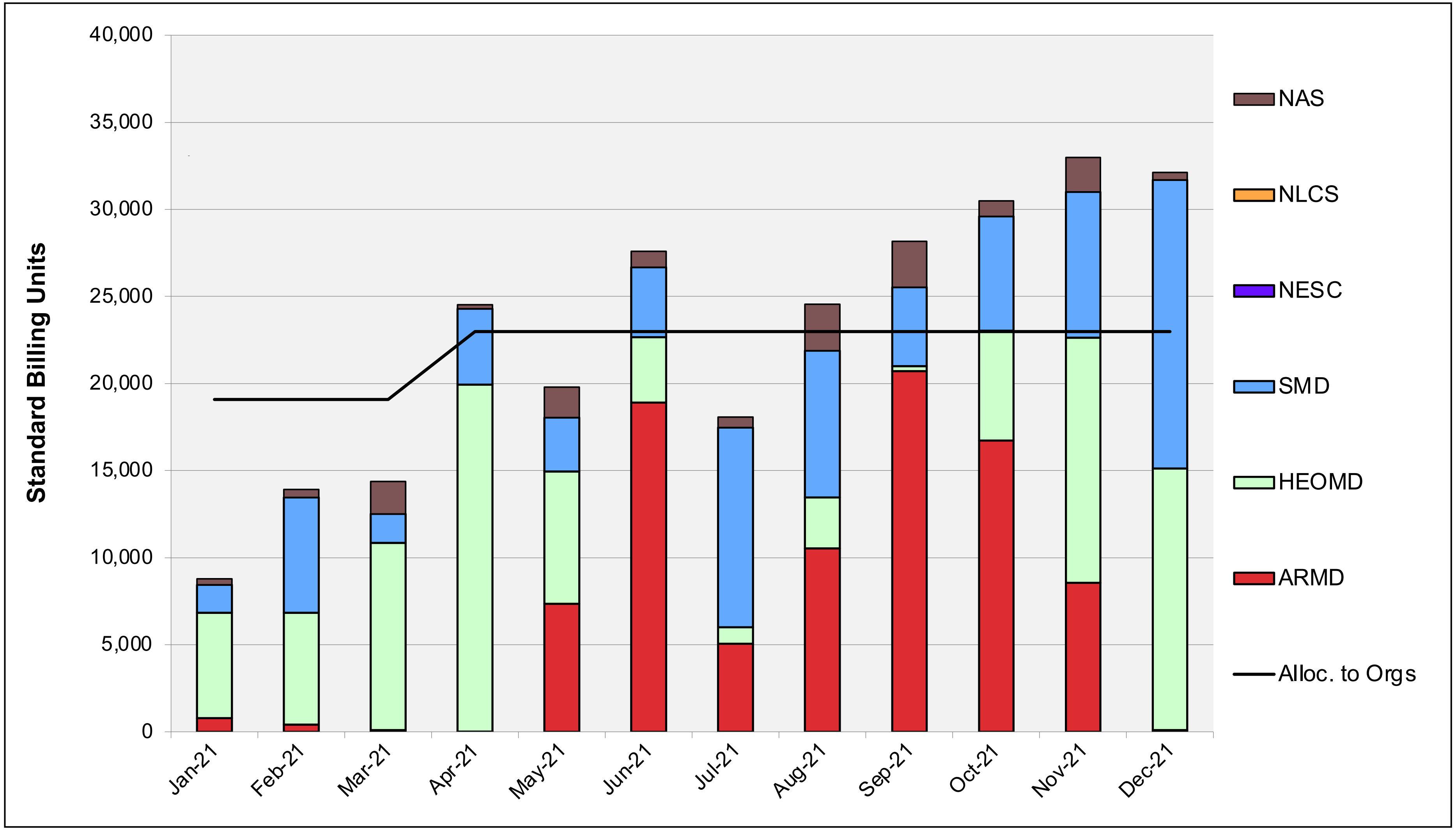
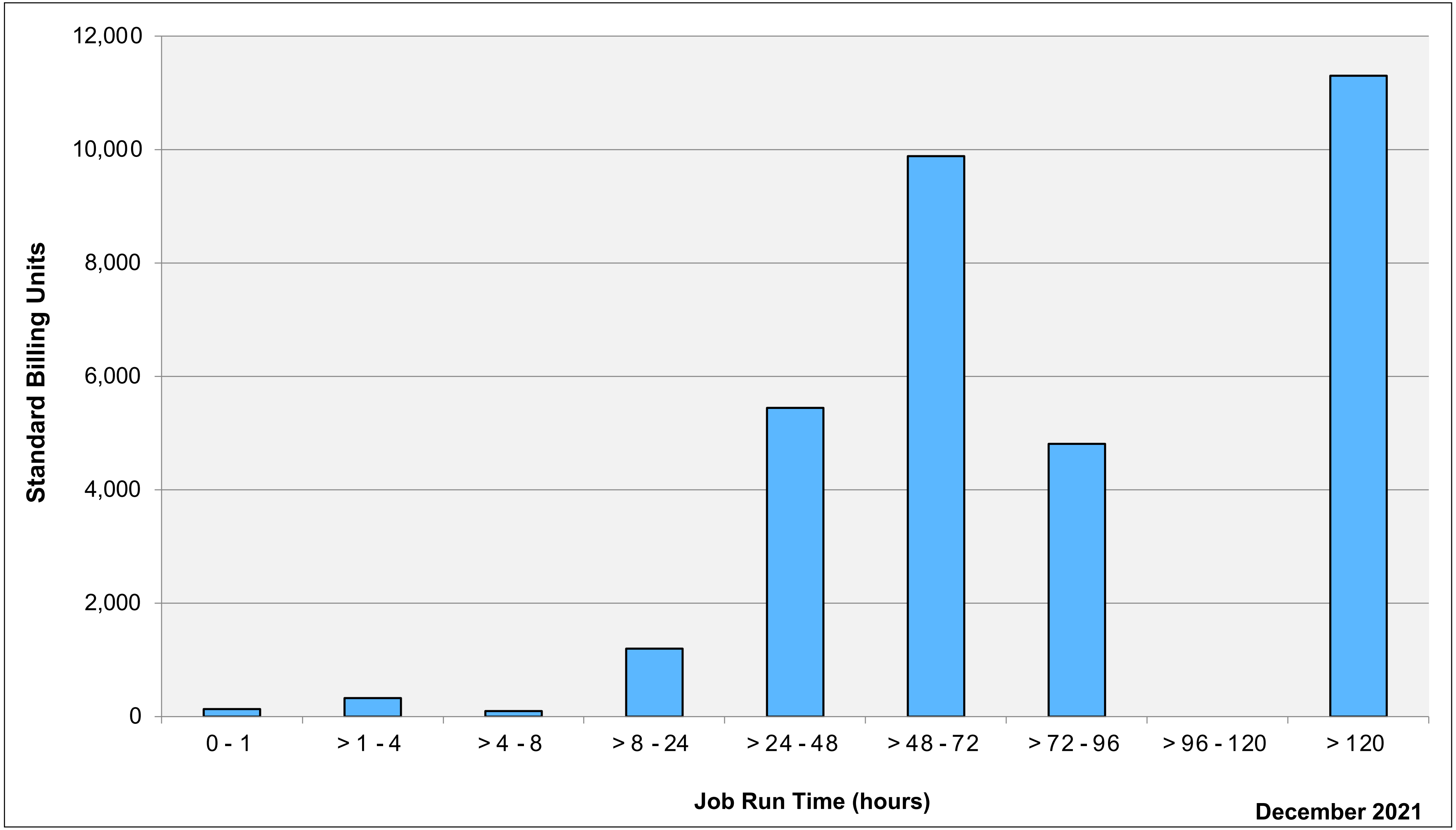


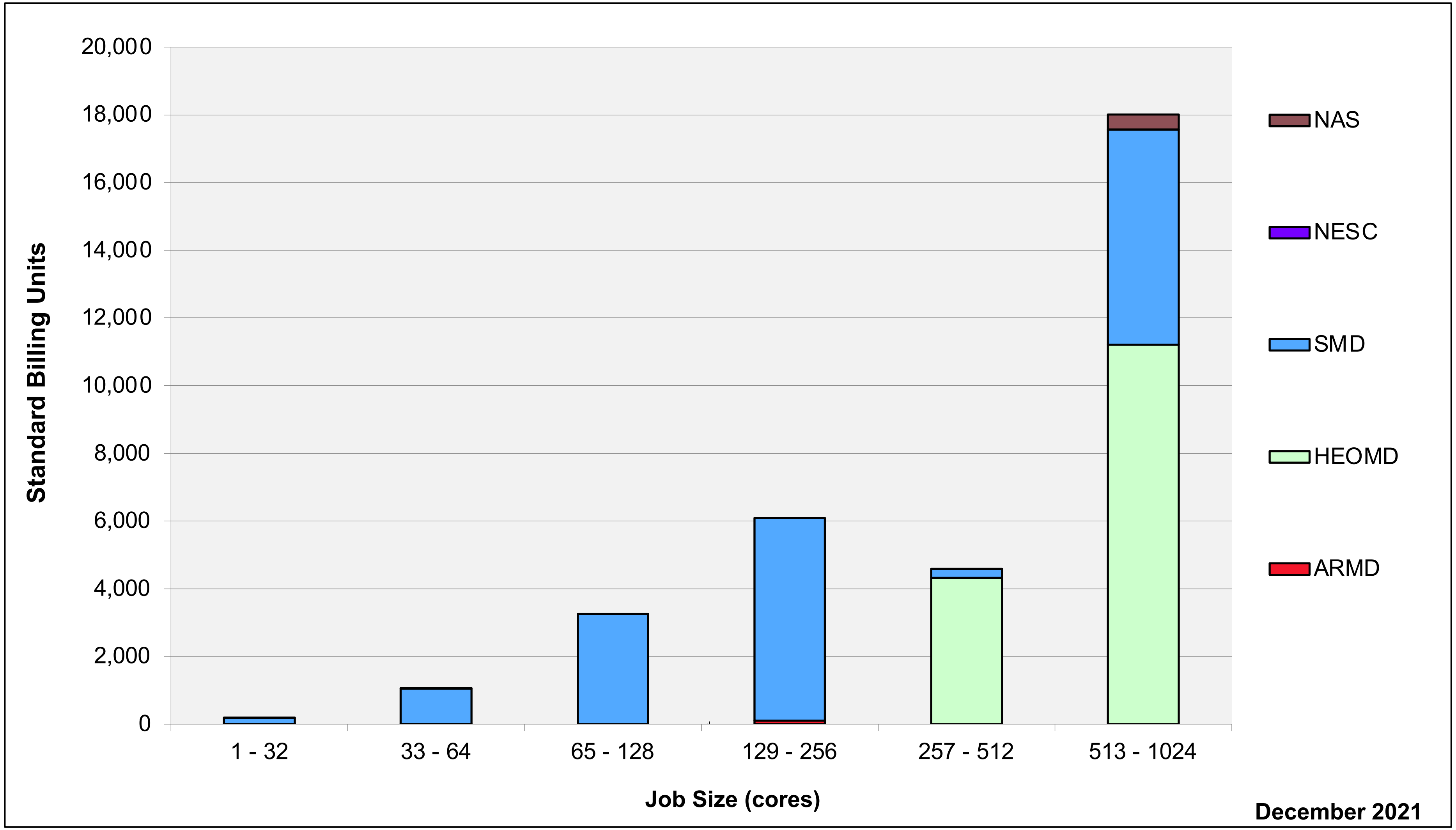
Endeavour: SBUs Reported, Normalized to 30-Day Month



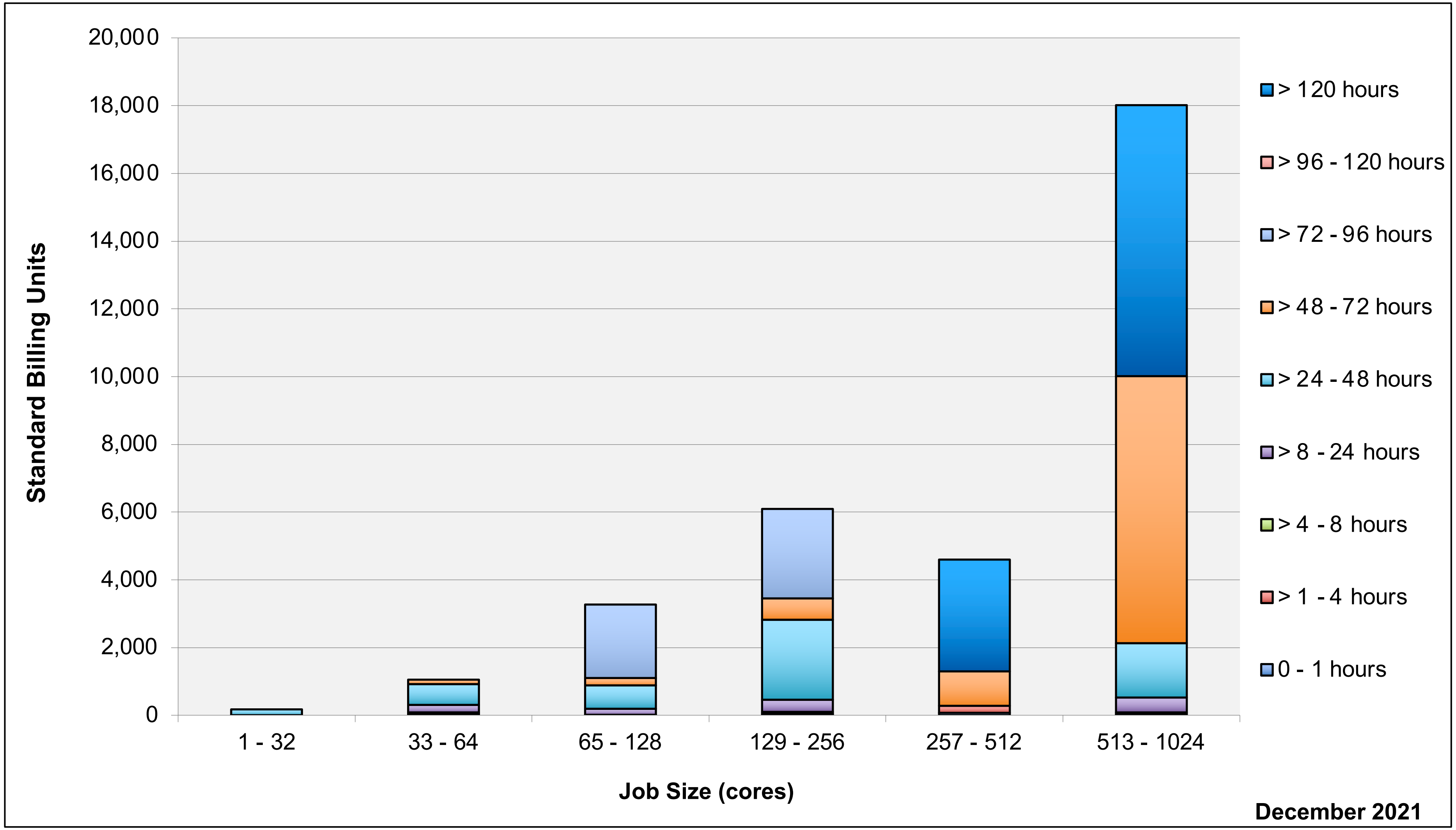
Endeavour: Monthly Utilization by Job Length



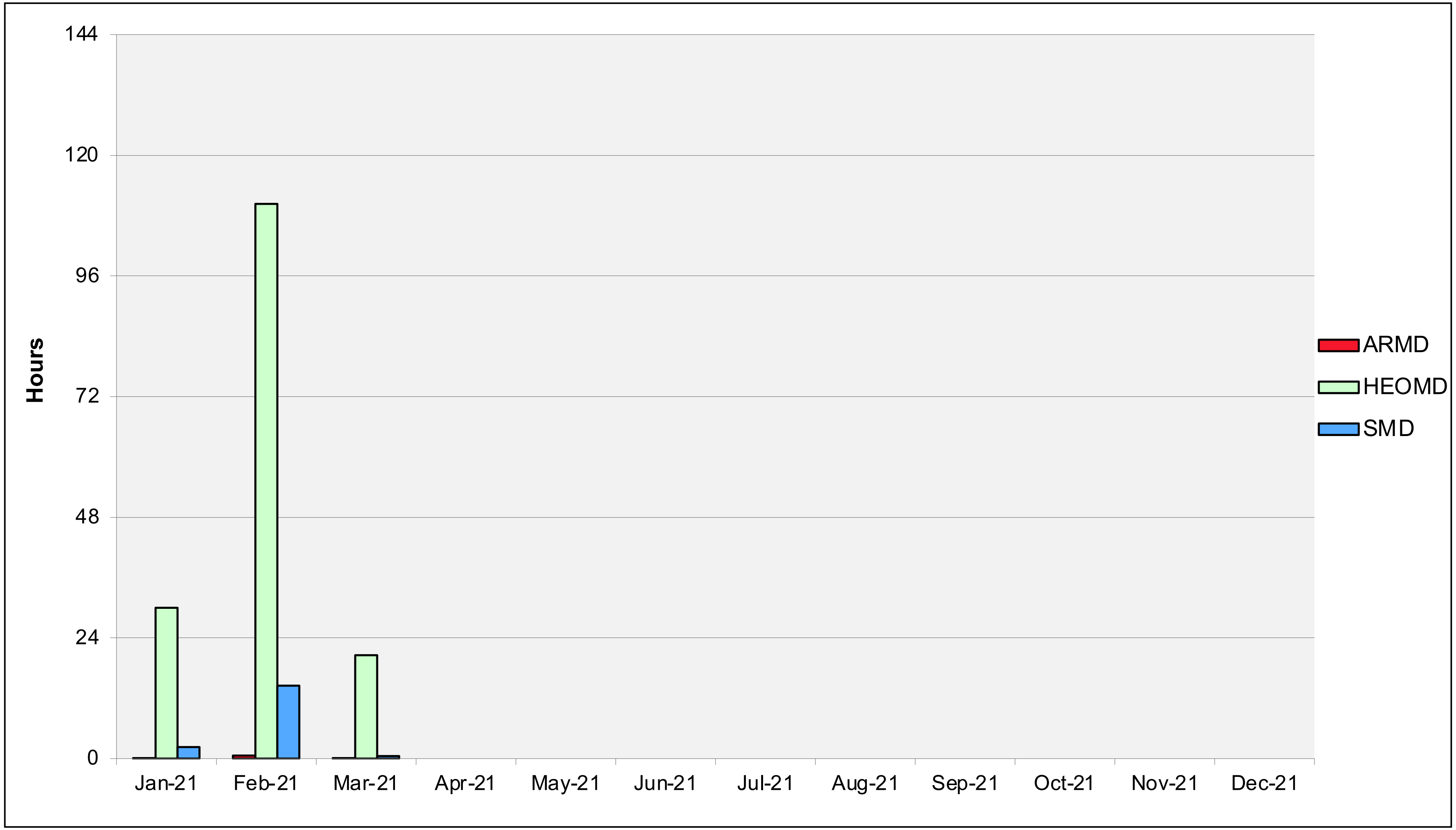
Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor